Search history


```
=> d his full

     (FILE 'HOME' ENTERED AT 13:31:33 ON 26 MAY 2006)

     FILE 'STNGUIDE' ENTERED AT 13:31:55 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 13:32:50 ON 26 MAY 2006

     FILE 'STNGUIDE' ENTERED AT 13:33:31 ON 26 MAY 2006
                SET LINE 250
                SET DETAIL OFF
                DIS SAVED/S
                SET LINE LOGIN
                SET DETAIL LOGIN

     FILE 'HCAPLUS' ENTERED AT 13:34:25 ON 26 MAY 2006
                ACT NWA377APP/A
                ---------
L1              1 SEA ABB=ON  PLU=ON  US2005-521377 /APPS
                ---------

     FILE 'REGISTRY' ENTERED AT 13:34:38 ON 26 MAY 2006
                ACT NWA377RNS/A
                ---------
L2              5 SEA ABB=ON  PLU=ON  (10605-40-0/BI OR 1066-35-9/BI OR 107-05-1/
                  BI OR 111-78-4/BI OR 12112-67-3/BI)
                ---------
                ACT NWA377IR/A
                ---------
L3          47943 SEA ABB=ON  PLU=ON  IR>0
                ---------
                ACT NWA377IR2/A
                ---------
L4           7579 SEA ABB=ON  PLU=ON  IR>1
                ---------
                ACT NWA377BATCH/A
                ---------
L5                STR
L6         428852 SEA SSS FUL L5
                ---------

     FILE 'HCAPLUS' ENTERED AT 13:37:55 ON 26 MAY 2006
                ACT NWA377IR2CAT/A
                ---------
L7   (       7579)SEA ABB=ON  PLU=ON  IR>1
L8            725 SEA ABB=ON  PLU=ON  L7/CAT
                ---------

     FILE 'STNGUIDE' ENTERED AT 13:38:08 ON 26 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 13:39:45 ON 26 MAY 2006

     FILE 'STNGUIDE' ENTERED AT 13:40:08 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 13:42:50 ON 26 MAY 2006
L9                STRUCTURE UPLOADED
L10             50 SEA SUB=L6 SSS SAM L9
L11         424806 SEA SUB=L6 SSS FUL L9
                DELETE DAV244PSTRA/A
                DELETE DAV244PSTRP/A
```

```
                DELETE DAV244PSTRQ/A
                DELETE OWE120AOLD/A
                DELETE OWE120NOTOLD/A
                DELETE OWE120UBIQ/A

     FILE 'STNGUIDE' ENTERED AT 13:47:26 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:25:23 ON 26 MAY 2006
L12         4046 SEA ABB=ON  PLU=ON  L6 NOT L11

     FILE 'HCAPLUS' ENTERED AT 14:26:04 ON 26 MAY 2006
L13      2857503 SEA ABB=ON  PLU=ON  (RACT OR RCT OR RGT)/RL
L*** DEL     683 S L13 AND L8

     FILE 'STNGUIDE' ENTERED AT 14:29:52 ON 26 MAY 2006

     FILE 'STNGUIDE' ENTERED AT 14:31:27 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:32:00 ON 26 MAY 2006
L14              STRUCTURE UPLOADED
L15           12 SEA SUB=L6 SSS SAM L14
L16         5231 SEA SUB=L6 SSS FUL L14
                 SAVE TEMP L16 NWA377STRD/A

     FILE 'HCAPLUS' ENTERED AT 14:34:16 ON 26 MAY 2006
L17         9286 SEA ABB=ON  PLU=ON  L16 (L) L13
L18           39 SEA ABB=ON  PLU=ON  L17 AND L8
                 SEL RN L18

     FILE 'REGISTRY' ENTERED AT 14:36:32 ON 26 MAY 2006
L19          837 SEA ABB=ON  PLU=ON  (12112-67-3/BI OR 617-86-7/BI OR 1066-35-9/
                 BI OR 107-05-1/BI OR 766-77-8/BI OR 10605-40-0/BI OR 18827-81-1
                 /BI OR 603-35-0/BI OR 998-30-1/BI OR 29681-57-0/BI OR 7440-05-3
                 /BI OR 7440-06-4/BI OR 111-78-4/BI OR 12246-51-4/BI OR
                 15243-33-1/BI OR 108-94-1/BI OR 12092-47-6/BI OR 14694-95-2/BI
                 OR 2031-62-1/BI OR 2487-90-3/BI OR 592-41-6/BI OR 7440-18-8/BI
                 OR 789-25-3/BI OR 98-86-2/BI OR 100-42-5/BI OR 100-52-7/BI OR
                 10210-68-1/BI OR 1079-66-9/BI OR 12111-11-4/BI OR 12148-71-9/BI
                  OR 13938-94-8/BI OR 14857-34-2/BI OR 16941-92-7/BI OR
                 4342-22-7/BI OR 498-66-8/BI OR 536-74-3/BI OR 603-32-7/BI OR
                 64-17-5/BI OR 693-02-7/BI OR 7439-88-5/BI OR 7440-04-2/BI OR
                 776-76-1/BI OR 930-68-7/BI OR 10025-78-2/BI OR 10170-69-1/BI
                 OR 1038-95-5/BI OR 104-53-0/BI OR 106-95-6/BI OR 1081-97-6/BI
                 OR 109-89-7/BI OR 110-54-3/BI OR 1192-62-7/BI OR 12080-32-9/BI
                 OR 12245-73-7/BI OR 123-72-8/BI OR 13269-52-8/BI OR 13829-48-6/
                 BI OR 13829-50-0/BI OR 14221-01-3/BI OR 1438-82-0/BI OR
                 1445-91-6/BI OR 146139-33-5/BI OR 14871-41-1/BI OR 148991-61-1/
                 BI OR 14996-61-3/BI OR 1517-69-7/BI OR 15696-40-9/BI OR
                 16941-12-1/BI OR 17685-52-8/BI OR 17718-70-6/BI OR 21693-13-0/B
                 I OR 220800-76-0/BI OR 220800-77-1/BI OR 220800-78-2/BI OR
                 220800-79-3/BI OR 24636-31-5/BI OR 2530-87-2/BI OR 25360-32-1/B
                 I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
                 /BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
                 BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
                 565-80-0/BI OR 583-60-8/BI OR 60255-04-1/BI OR 60255-25-6/BI
                 OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
                 OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
                 656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
                 I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
                 75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/
```

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L20          222 SEA ABB=ON  PLU=ON  L19 AND L11

     FILE 'HCAPLUS' ENTERED AT 14:38:23 ON 26 MAY 2006
L21         2871 SEA ABB=ON  PLU=ON  L20 (L) PREP/RL
L22           32 SEA ABB=ON  PLU=ON  L18 AND L21
L23       405200 SEA ABB=ON  PLU=ON  (?ALKENE? OR ?DIENE?)/BI
L24           19 SEA ABB=ON  PLU=ON  L22 AND L23
L*** DEL   44857 S (SINGLE STEP?)/BI OR (ONE STEP?)/BI OR (1 STEP)/BI
L25       793758 SEA ABB=ON  PLU=ON  CONTINU?/BI
L26            2 SEA ABB=ON  PLU=ON  L22 AND L25

     FILE 'CASREACT' ENTERED AT 14:44:42 ON 26 MAY 2006
L27          334 SEA ABB=ON  PLU=ON  L4/CAT
                 D COST

     FILE 'STNGUIDE' ENTERED AT 14:45:43 ON 26 MAY 2006

     FILE 'CASREACT' ENTERED AT 14:51:01 ON 26 MAY 2006
L28         5265 SEA ABB=ON  PLU=ON  L16/RRT
L29           24 SEA ABB=ON  PLU=ON  L28 (L) L27

     FILE 'HCAPLUS' ENTERED AT 14:52:59 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:53:25 ON 26 MAY 2006
L30         3438 SEA ABB=ON  PLU=ON  L4 AND X>0

     FILE 'HCAPLUS' ENTERED AT 14:53:44 ON 26 MAY 2006
L31          517 SEA ABB=ON  PLU=ON  L30 (L) CAT/RL
L*** DEL       0 S L17 (L) L31
L32           23 SEA ABB=ON  PLU=ON  L17 AND L31 AND L21

     FILE 'STNGUIDE' ENTERED AT 14:57:10 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:57:38 ON 26 MAY 2006
L33       165275 SEA ABB=ON  PLU=ON  L11 AND CASREACT/LC

     FILE 'STNGUIDE' ENTERED AT 14:58:44 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 15:02:04 ON 26 MAY 2006
L34              STRUCTURE UPLOADED
L35           50 SEA SUB=L6 SSS SAM L34

     FILE 'STNGUIDE' ENTERED AT 15:03:11 ON 26 MAY 2006

     FILE 'CASREACT' ENTERED AT 15:04:44 ON 26 MAY 2006

     FILE 'STNGUIDE' ENTERED AT 15:05:10 ON 26 MAY 2006

     FILE 'CASREACT' ENTERED AT 15:07:34 ON 26 MAY 2006
L36              STRUCTURE UPLOADED
L37           29 SEA SSS SAM L36 (  1513 REACTIONS)

     FILE 'STNGUIDE' ENTERED AT 15:08:14 ON 26 MAY 2006

     FILE 'CASREACT' ENTERED AT 15:12:09 ON 26 MAY 2006
L38              STRUCTURE UPLOADED
L39            4 SEA SSS SAM L38 (    49 REACTIONS)
                 D STAT QUE L37
                 D STAT QUE L39
L40              STRUCTURE UPLOADED
```

```
L41           4 SEA SSS SAM L40 (    37 REACTIONS)

     FILE 'STNGUIDE' ENTERED AT 15:17:01 ON 26 MAY 2006
                D SCA

     FILE 'HCAPLUS' ENTERED AT 15:18:04 ON 26 MAY 2006
L42           24 SEA ABB=ON  PLU=ON  L29
L43           16 SEA ABB=ON  PLU=ON  L22 AND L42
L44           12 SEA ABB=ON  PLU=ON  L32 AND L42

     FILE 'CASREACT' ENTERED AT 15:20:56 ON 26 MAY 2006
                D SCA L29
                SEL RX L29
                DELETE SELECT
                SEL RX L29

     FILE 'REGISTRY' ENTERED AT 15:29:43 ON 26 MAY 2006
                EDIT  E1-E262 RX RN
L45          262 SEA ABB=ON  PLU=ON  (75-09-2/RN OR 7732-18-5/RN OR 107-06-2/RN
                OR 12112-67-3/RN OR 109-99-9/RN OR 110-54-3/RN OR 67-56-1/RN
                OR 617-86-7/RN OR 760-32-7/RN OR 501419-01-8/RN OR 144-55-8/RN
                OR 501419-19-8/RN OR 501419-20-1/RN OR 501419-21-2/RN OR
                603-35-0/RN OR 501419-22-3/RN OR 75-05-8/RN OR 108-48-5/RN OR
                12246-51-4/RN OR 501419-23-4/RN OR 69739-34-0/RN OR 185346-09-2
                /RN OR 96-33-3/RN OR 501419-02-9/RN OR 18827-81-1/RN OR
                501419-08-5/RN OR 501419-27-8/RN OR 7647-01-0/RN OR 1191-15-7/R
                N OR 121289-23-4/RN OR 501419-10-9/RN OR 304-59-6/RN OR
                501419-28-9/RN OR 108-94-1/RN OR 87413-09-0/RN OR 108-88-3/RN
                OR 501419-29-0/RN OR 558-13-4/RN OR 60-29-7/RN OR 74-88-4/RN
                OR 109-72-8/RN OR 12125-02-9/RN OR 584-08-7/RN OR 37342-97-5/RN
                 OR 56-23-5/RN OR 7553-56-2/RN OR 14221-01-3/RN OR 501419-06-3/
                RN OR 594-19-4/RN OR 7646-85-7/RN OR 1066-35-9/RN OR 1333-74-0/
                RN OR 429-41-4/RN OR 4342-22-7/RN OR 10605-40-0/RN OR 109389-69
                -7/RN OR 13810-04-3/RN OR 82499-43-2/RN OR 107-05-1/RN OR
                12148-71-9/RN OR 29681-57-0/RN OR 501419-32-5/RN OR 592-41-6/RN
                 OR 762-42-5/RN OR 930-68-7/RN OR 4419-18-5/RN OR 616-47-7/RN
                OR 630-08-0/RN OR 84-58-2/RN OR 96474-45-2/RN OR 101-02-0/RN
                OR 121-44-8/RN OR 124-63-0/RN OR 501419-33-6/RN OR 111-78-4/RN
                OR 123-91-1/RN OR 603-32-7/RN OR 71195-85-2/RN OR 7664-39-3/RN
                OR 109-89-7/RN OR 501419-34-7/RN OR 64-17-5/RN OR 70790-00-0/RN
                 OR 75-03-6/RN OR 110-82-7/RN OR 151-50-8/RN OR 168557-46-8/RN
                OR 513-81-5/RN OR 598-30-1/RN OR 7782-44-7/RN OR 107-30-2/RN
                OR 111-66-0/RN OR 13508-63-9/RN OR 168557-50-4/RN OR 168557-53-
                7/RN OR 2227-29-4/RN OR 40962-02-5/RN OR 501419-30-3/RN OR
                57-14-7/RN OR 627-19-0/RN OR 68928-07-4/RN OR 68928-08-5/RN OR
                7087-68-5/RN OR 998-30-1/RN OR 100-42-5/RN OR 100-52-7/RN OR
                10175-53-8/RN OR 1192-62-7/RN OR 123-72-8/RN OR 162157-02-0/RN
                OR 168557-47-9/RN OR

     FILE 'CASREACT' ENTERED AT 15:31:34 ON 26 MAY 2006
L46        12591 SEA ABB=ON  PLU=ON  L45/PRO
L47           24 SEA ABB=ON  PLU=ON  L29 (L) L46

     FILE 'HCAPLUS' ENTERED AT 15:34:40 ON 26 MAY 2006

     FILE 'STNGUIDE' ENTERED AT 15:34:55 ON 26 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 15:36:42 ON 26 MAY 2006
L48            1 SEA ABB=ON  PLU=ON  L1 AND L22
L49           12 SEA ABB=ON  PLU=ON  KORNEK T?/AU
```

```
L50         1132 SEA ABB=ON  PLU=ON  BAUER A?/AU
L51            1 SEA ABB=ON  PLU=ON  SENDEN D?/AU
L52            1 SEA ABB=ON  PLU=ON  (L49 AND (L50 OR L51)) OR (L50 AND L51)
L53            2 SEA ABB=ON  PLU=ON  (L49 OR L50 OR L51) AND (L22 OR L24 OR L26
                 OR L32)

     FILE 'CASREACT' ENTERED AT 15:38:22 ON 26 MAY 2006
L54            8 SEA ABB=ON  PLU=ON  KORNEK T?/AU
L55           33 SEA ABB=ON  PLU=ON  BAUER A?/AU
L56            1 SEA ABB=ON  PLU=ON  SENDEN D?/AU
L57            1 SEA ABB=ON  PLU=ON  (L54 AND (L55 OR L56)) OR (L55 AND L56)
L58            2 SEA ABB=ON  PLU=ON  (L54 OR L55 OR L56) AND L47

     FILE 'STNGUIDE' ENTERED AT 15:40:40 ON 26 MAY 2006

     FILE 'REGISTRY' ENTERED AT 15:44:49 ON 26 MAY 2006
                 D STAT QUE L6
                 D STAT QUE L11
                 D STAT QUE L16

     FILE 'HCAPLUS' ENTERED AT 15:45:34 ON 26 MAY 2006
                 D QUE NOS L52
                 D QUE NOS L53
L59            2 SEA ABB=ON  PLU=ON  L52 OR L53

     FILE 'CASREACT' ENTERED AT 15:46:49 ON 26 MAY 2006
                 D QUE NOS L57
                 D QUE NOS L58
L60            2 SEA ABB=ON  PLU=ON  L57 OR L58

     FILE 'HCAPLUS, CASREACT' ENTERED AT 15:47:25 ON 26 MAY 2006
L61            2 DUP REM L59 L60 (2 DUPLICATES REMOVED)
                       ANSWERS '1-2' FROM FILE HCAPLUS
                 D IBIB ABS HITIND HITSTR L61 1-2

     FILE 'STNGUIDE' ENTERED AT 15:48:20 ON 26 MAY 2006

     FILE 'CASREACT' ENTERED AT 15:50:26 ON 26 MAY 2006
                 D QUE NOS L47
L62           22 SEA ABB=ON  PLU=ON  L47 NOT L60

     FILE 'HCAPLUS' ENTERED AT 15:50:30 ON 26 MAY 2006
                 D QUE NOS L22
                 D QUE NOS L24
                 D QUE NOS L26
                 D QUE NOS L32
L63           30 SEA ABB=ON  PLU=ON  (L22 OR L24 OR L26 OR L32) NOT L59

     FILE 'CASREACT, HCAPLUS' ENTERED AT 15:50:58 ON 26 MAY 2006
L64           38 DUP REM L62 L63 (14 DUPLICATES REMOVED)
                       ANSWERS '1-22' FROM FILE CASREACT
                       ANSWERS '23-38' FROM FILE HCAPLUS
                 D IBIB ABS HIT L64 1-22
                 D IBIB ABS HITIND HITSTR L64 23-38


     FILE HOME

     FILE STNGUIDE
     FILE CONTAINS CURRENT INFORMATION.
```

LAST RELOADED: May 19, 2006 (20060519/UP).

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0
DICTIONARY FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE HCAPLUS

FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23
FILE LAST UPDATED: 25 May 2006 (20060525/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CASREACT

FILE CONTENT:1840 - 21 May 2006 VOL 144 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
**********************************************************
*                                                        *
*     CASREACT now has more than 10 million reactions    *
*                                                        *
**********************************************************
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

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=> file registry
FILE 'REGISTRY' ENTERED AT 15:44:49 ON 26 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   25 MAY 2006  HIGHEST RN 885654-58-0
DICTIONARY FILE UPDATES:  25 MAY 2006  HIGHEST RN 885654-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************************
*                                                                       *
* The CA roles and document type information have been removed from     *
* the IDE default display format and the ED field has been added,       *
* effective March 20, 2005.  A new display format, IDERL, is now        *
* available and contains the CA role and document type information.     *
*                                                                       *
*************************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

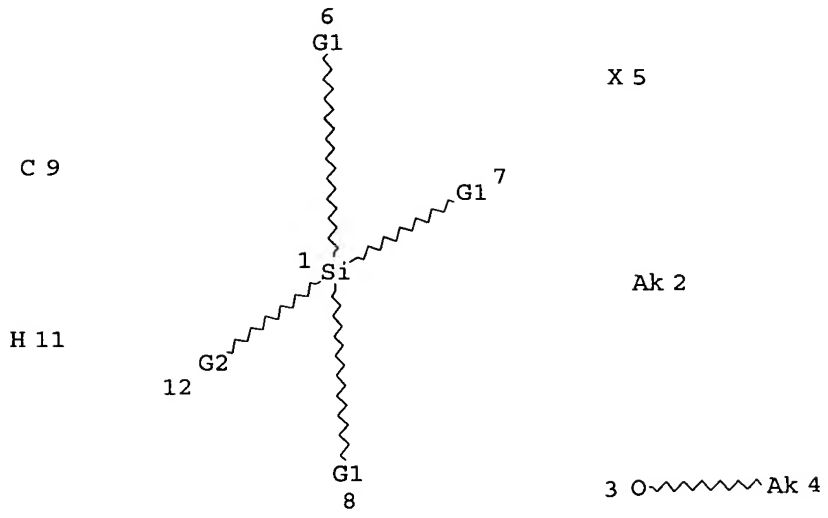
http://www.cas.org/ONLINE/UG/regprops.html

=> d stat que L6

L5              STR
```

STRUCTURE QUERIES

C 10




```
VAR G1=2/3/5
VAR G2=9/10/11
NODE ATTRIBUTES:
NSPEC    IS C       AT   1
NSPEC    IS C       AT   2
NSPEC    IS C       AT   3
NSPEC    IS C       AT   4
NSPEC    IS C       AT   5
NSPEC    IS C       AT   6
NSPEC    IS C       AT   7
NSPEC    IS C       AT   8
NSPEC    IS C       AT   9
NSPEC    IS R       AT  10
NSPEC    IS C       AT  11
NSPEC    IS C       AT  12
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS   AT   1  2  3  4  5  9 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L6        428852 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 1236316 ITERATIONS                    428852 ANSWERS
SEARCH TIME: 00.00.12


=> d stat que L11

L5              STR
```

=> □ CASREACT 1-22; HCAPLUS 23-38:

=> file casreact
FILE 'CASREACT' ENTERED AT 15:50:26 ON 26 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 21 May 2006 VOL 144 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

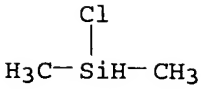
****
*
* CASREACT now has more than 10 million reactions
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

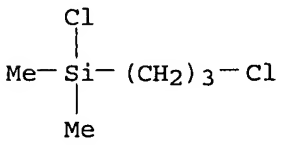
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que nos L47

L4 7579 SEA FILE=REGISTRY ABB=ON PLU=ON IR>1
L5 STR
L6 428852 SEA FILE=REGISTRY SSS FUL L5
L14 STR
L16 5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
L27 334 SEA FILE=CASREACT ABB=ON PLU=ON L4/CAT
L28 5265 SEA FILE=CASREACT ABB=ON PLU=ON L16/RRT
L29 24 SEA FILE=CASREACT ABB=ON PLU=ON L28 (L) L27
L45 262 SEA FILE=REGISTRY ABB=ON PLU=ON (75-09-2/RN OR 7732-18-5/RN OR 107-06-2/RN OR 12112-67-3/RN OR 109-99-9/RN OR 110-54-3/RN OR 67-56-1/RN OR 617-86-7/RN OR 760-32-7/RN OR 501419-01-8/RN OR 144-55-8/RN OR 501419-19-8/RN OR 501419-20-1/RN OR 501419-21-2/RN OR 603-35-0/RN OR 501419-22-3/RN OR 75-05-8/RN OR 108-48-5/RN OR 12246-51-4/RN OR 501419-23-4/RN OR 69739-34-0/RN OR 185346-09-2/RN OR 96-33-3/RN OR 501419-02-9/RN OR 18827-81-1/RN OR 501419-08-5/RN OR 501419-27-8/RN OR 7647-01-0/RN OR 1191-15-7/RN OR 121289-23-4/RN OR 501419-10-9/RN OR 304-59-6/RN OR 501419-28-9/RN OR 108-94-1/RN OR 87413-09-0/RN OR 108-88-3/RN OR 501419-29-0/RN OR 558-13-4/RN OR 60-29-7/RN OR 74-88-4/RN OR 109-72-8/RN OR 12125-02-9/RN OR 584-08-7/RN OR 37342-97-5/RN OR 56-23-5/RN OR 7553-56-2/RN OR 14221-01-3/RN OR 501419-06-3/RN OR 594-19-4/RN OR 7646-85-7/RN OR 1066-35-9/RN OR 1333-74-0/RN OR 429-41-4/RN OR 4342-22-7/RN OR 10605-40-0/RN OR 109389-69-7/RN OR 13810-04-3/RN OR 82499-43-2/RN OR 107-05-1/RN OR 12148-71-9/RN OR 29681-57-0/RN OR 501419-32-5/RN OR 592-41-6/RN OR 762-42-5/RN OR 930-68-7/RN OR 4419-18-5/RN OR 616-47-7/RN OR 630-08-0/RN OR 84-58-2/RN OR 96474-45-2/RN OR 101-02-0/RN OR 121-44-8/RN OR 124-63-0/RN OR 501419-33-6/RN OR

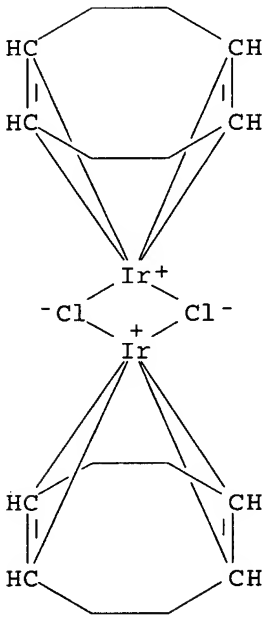


IT **10605-40-0P**, Chloro(3-chloropropyl)dimethylsilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 10605-40-0 HCAPLUS
CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



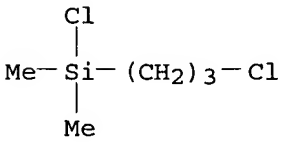
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CC 29-6 (Organometallic and Organometalloidal Compounds)
ST organo silane prepn; iridium catalyzed hydrosilylation **alkene** hydrosilane; platinum catalyzed hydrosilylation **alkene** hydrosilane
IT Hydrosilylation catalysts
(preparation of organosilanes via **diene** iridium chloride catalyzed hydrosilylation of **alkenes** with hydrosilanes)
IT **12112-67-3** 134588-15-1
RL: **CAT (Catalyst use)**; USES (Uses)
(hydrosilylation of allyl chloride with chlorodimethylsilane catalyzed with)
IT **1066-35-9**, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(iridium catalyzed hydrosilylation of allyl chloride with)
IT 111-78-4, 1,5-**Cyclooctadiene**
RL: CAT (Catalyst use); USES (Uses)
(iridium catalyzed hydrosilylation of allyl chloride with chlorodimethylsilane in presence of)
IT **10605-40-0P**, Chloro(3-chloropropyl)dimethylsilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **12112-67-3**
RL: **CAT (Catalyst use)**; USES (Uses)
(hydrosilylation of allyl chloride with chlorodimethylsilane catalyzed with)
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



IT **1066-35-9**, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(iridium catalyzed hydrosilylation of allyl chloride with)
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

IT **10605-40-0P**, Chloro(3-chloropropyl)dimethylsilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)
RN 10605-40-0 HCAPLUS
CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2002:51103 HCAPLUS
DOCUMENT NUMBER: 136:102512
TITLE: Preparation of organosilanes via transition metal catalyzed hydrosilylation of **alkenes**
INVENTOR(S): Schaefer, Oliver; Frey, Volker; Pachaly, Bernd; **Bauer, Andreas**; Kriegbaum, Markus; Brader, Leonhard
PATENT ASSIGNEE(S): Consortium fuer Elektrochemische Industrie Gmbh, Germany
SOURCE: Ger., 4 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10053037	C1	20020117	DE 2000-10053037	20001026
EP 1201671	A1	20020502	EP 2001-118869	20010816
EP 1201671	B1	20031112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002052520	A1	20020502	US 2001-966822	20010927
US 6388119	B2	20020514		
JP 2002179684	A2	20020626	JP 2001-324905	20011023
CN 1351015	A	20020529	CN 2001-136677	20011024

PRIORITY APPLN. INFO.: DE 2000-10053037 A 20001026
OTHER SOURCE(S): CASREACT 136:102512; MARPAT 136:102512
AB The preparation of organosilanes, R6R5CHCHR4SiR1R2R3 (R1-R3 = Si-C bonded halo substituted C1-18 hydrocarbon, Cl, C1-18 alkoxy, etc.; R4-R6 = H, F, Cl, alkoxy, organoamino, CN, NCO substituted C1-18 hydrocarbon, chloro-, fluoro-C1-18 alkoxy, cyclic, etc.), via [(**diene**)IrCl]2-catalyzed hydrosilylation of R5R6CH:CHR4 with HSiR1R2R3, is described. Thus, di-μ-chlorobis[(**cyclooctadiene**)iridium]/1,5-**cyclooctadiene**-catalyzed hydrosilylation of allyl chloride with chlorodimethylsilane gave 95% chloro(3-chloropropyl)dimethylsilane.
IC ICM C07F007-12
ICS C07F007-08; C07F007-10; C07F007-18

(organo-; **continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

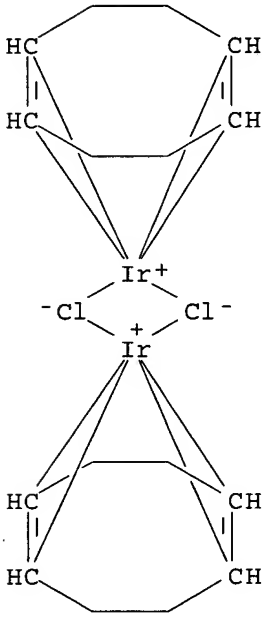
IT 111-78-4, 1,5-**Cyclooctadiene 12112-67-3**, Bis[chloro(1,5-**cyclooctadiene**)iridium]
RL: **CAT (Catalyst use)**; USES (Uses)
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

IT 107-05-1, Allyl chloride **1066-35-9**, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

IT **10605-40-0P**, Chloro(3-chloropropyl)dimethylsilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

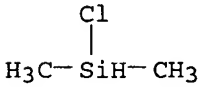
IT **12112-67-3**, Bis[chloro(1,5-**cyclooctadiene**)iridium]
RL: **CAT (Catalyst use)**; USES (Uses)
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



IT **1066-35-9**, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)

RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



PROCESSING COMPLETED FOR L60
L61 2 DUP REM L59 L60 (2 DUPLICATES REMOVED)
ANSWERS '1-2' FROM FILE HCAPLUS

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L61 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2003:811648 HCAPLUS
DOCUMENT NUMBER: 139:292356
TITLE: **Continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane
INVENTOR(S): **Kornek, Thomas**; **Bauer, Andreas**; **Senden, Diana**
PATENT ASSIGNEE(S): Wacker-Chemie GmbH, Germany
SOURCE: Ger., 4 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10232663	C1	20031016	DE 2002-10232663	20020718
WO 2004009607	A1	20040129	WO 2003-EP6204	20030612
W: CN, JP, PL, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1530575	A1	20050518	EP 2003-735613	20030612
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1668624	A	20050914	CN 2003-817180	20030612
JP 2005533123	T2	20051104	JP 2004-522176	20030612
US 2005240043	A1	20051027	US 2005-521377	20050118
PRIORITY APPLN. INFO.:			DE 2002-10232663 A	20020718
			WO 2003-EP6204 W	20030612

OTHER SOURCE(S): CASREACT 139:292356; MARPAT 139:292356
AB Procedure for the **continuous** production of silane, R6R5CHR4CHSiR1R2R3 (R1-R3 = C1-18 hydrocarbyl, Cl, C1-18 alkoxy, etc.; R4-R6 = H, F, Cl, alkoxy, amino, cyano, NCO, C1-18 hydrocarbyl, etc.), via [(**diene**)IrCl]2-catalyzed reaction of silane HSiR1R2R3 with **alkene** R6R5CH:CHR4 and free **diene** as cocatalyst is described. [(cod)IrCl]2. The reaction temperature 30-200° and the reaction pressure 0.11-50.0 Mpa.
IC ICM C07F007-12
ICS C07F007-08; C07F007-10; C07F007-18
CC 29-6 (Organometallic and Organometalloidal Compounds)
ST organo silane prepn; iridium **diene** halide catalyzed addn silane **alkene**
IT Addition reaction
Addition reaction catalysts
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)
IT **Alkenes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**continuous** preparation of organosilanes via iridium catalyzed reaction of **alkene** with silane)
IT Silanes
RL: SPN (Synthetic preparation); PREP (Preparation)

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L28         5265 SEA FILE=CASREACT ABB=ON  PLU=ON  L16/RRT
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                 616-47-7/RN OR 630-08-0/RN OR 84-58-2/RN OR 96474-45-2/RN OR
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                 7664-39-3/RN OR 109-89-7/RN OR 501419-34-7/RN OR 64-17-5/RN OR
                 70790-00-0/RN OR 75-03-6/RN OR 110-82-7/RN OR 151-50-8/RN OR
                 168557-46-8/RN OR 513-81-5/RN OR 598-30-1/RN OR 7782-44-7/RN
                 OR 107-30-2/RN OR 111-66-0/RN OR 13508-63-9/RN OR 168557-50-4/R
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L55           33 SEA FILE=CASREACT ABB=ON  PLU=ON  BAUER A?/AU
L56            1 SEA FILE=CASREACT ABB=ON  PLU=ON  SENDEN D?/AU
L58            2 SEA FILE=CASREACT ABB=ON  PLU=ON  (L54 OR L55 OR L56) AND L47

=> s L57 or L58
L60            2 L57 OR L58

=> dup rem L59 L60
FILE 'HCAPLUS' ENTERED AT 15:47:25 ON 26 MAY 2006
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PROCESSING COMPLETED FOR L59
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                OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
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L21          2871 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 (L) PREP/RL
L22            32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L21
L23        405200 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (?ALKENE? OR ?DIENE?)/BI
L24            19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L23
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L26             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L25
L30          3438 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND X>0
L31           517 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 (L) CAT/RL
L32            23 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L31 AND L21
L49            12 SEA FILE=HCAPLUS ABB=ON  PLU=ON  KORNEK T?/AU
L50          1132 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BAUER A?/AU
L51             1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  SENDEN D?/AU
L53             2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L49 OR L50 OR L51) AND (L22
                  OR L24 OR L26 OR L32)


=> s L52 or L53
L59             2 L52 OR L53

=> file casreact
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FILE CONTENT:1840 - 21 May 2006 VOL 144 ISS 21

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*     CASREACT now has more than 10 million reactions      *
*                                                          *
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

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L56             1 SEA FILE=CASREACT ABB=ON  PLU=ON  SENDEN D?/AU
L57             1 SEA FILE=CASREACT ABB=ON  PLU=ON  (L54 AND (L55 OR L56)) OR
                  (L55 AND L56)
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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23
FILE LAST UPDATED: 25 May 2006 (20060525/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L9              STR
L11      424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
L13     2857503 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (RACT OR RCT OR RGT)/RL
L14             STR
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               I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
               /BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
               BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
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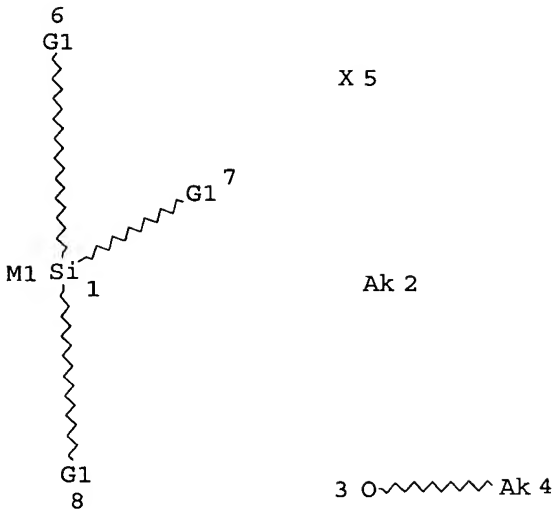

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NSPEC IS C AT 1
NSPEC IS C AT 2
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NSPEC IS C AT 8
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 1 2 3 4 5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 428849 ITERATIONS 5231 ANSWERS
SEARCH TIME: 00.00.05

=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 15:45:34 ON 26 MAY 2006
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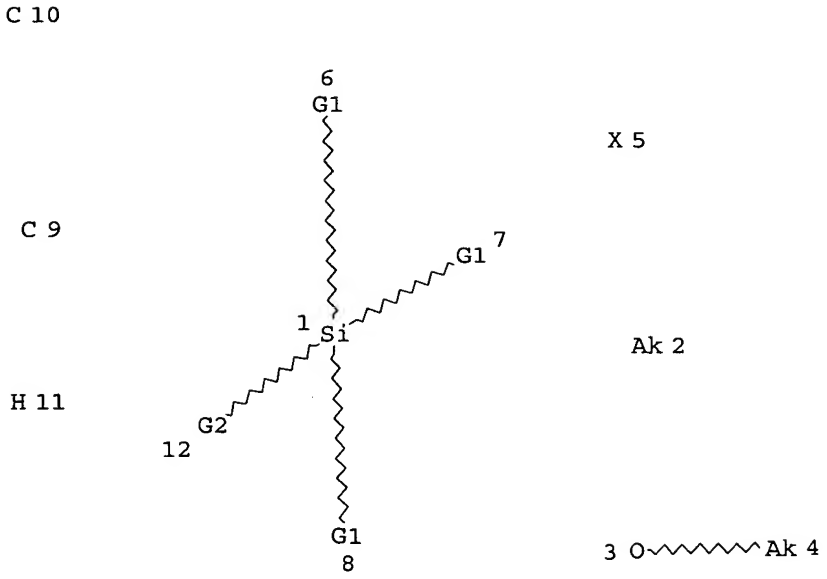
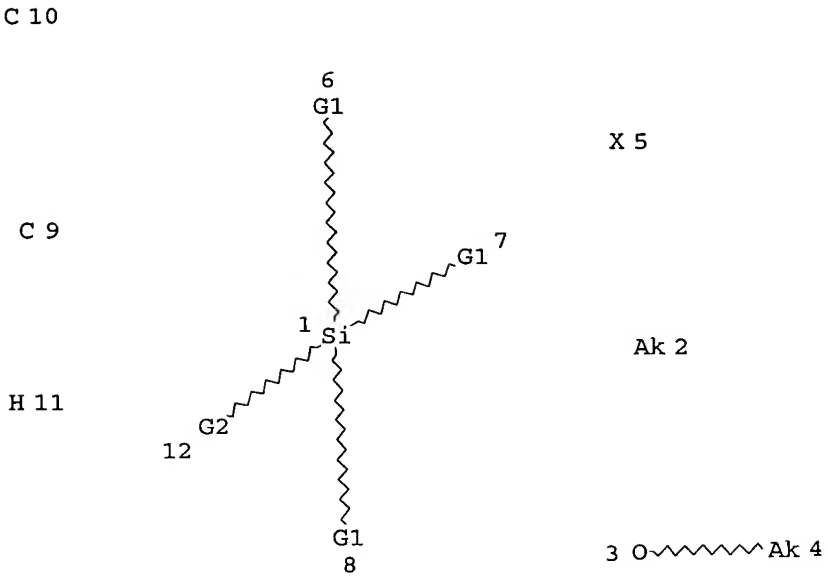
AUTHOR SEARCH




```
VAR G1=2/3/5
VAR G2=9/10/11
NODE ATTRIBUTES:
NSPEC    IS C       AT    1
NSPEC    IS C       AT    2
NSPEC    IS C       AT    3
NSPEC    IS C       AT    4
NSPEC    IS C       AT    5
NSPEC    IS C       AT    6
NSPEC    IS C       AT    7
NSPEC    IS C       AT    8
NSPEC    IS C       AT    9
NSPEC    IS R       AT   10
NSPEC    IS C       AT   11
NSPEC    IS C       AT   12
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS   AT    1  2  3  4  5  9 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L6        428852 SEA FILE=REGISTRY SSS FUL L5
L14              STR
```




```
VAR G1=2/3/5
VAR G2=9/10/11
NODE ATTRIBUTES:
NSPEC   IS C      AT   1
NSPEC   IS C      AT   2
NSPEC   IS C      AT   3
NSPEC   IS C      AT   4
NSPEC   IS C      AT   5
NSPEC   IS C      AT   6
NSPEC   IS C      AT   7
NSPEC   IS C      AT   8
NSPEC   IS C      AT   9
NSPEC   IS R      AT  10
NSPEC   IS C      AT  11
NSPEC   IS C      AT  12
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   1  2  3  4  5  9 11
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
L6       428852 SEA FILE=REGISTRY SSS FUL L5
L9              STR
L11      424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9

100.0% PROCESSED  428456 ITERATIONS                      424806 ANSWERS
SEARCH TIME: 00.00.05


=> d stat que L16

L5              STR
```

```
                111-78-4/RN OR 123-91-1/RN OR 603-32-7/RN OR 71195-85-2/RN OR
                7664-39-3/RN OR 109-89-7/RN OR 501419-34-7/RN OR 64-17-5/RN OR
                70790-00-0/RN OR 75-03-6/RN OR 110-82-7/RN OR 151-50-8/RN OR
                168557-46-8/RN OR 513-81-5/RN OR 598-30-1/RN OR 7782-44-7/RN
                OR 107-30-2/RN OR 111-66-0/RN OR 13508-63-9/RN OR 168557-50-4/R
                N OR 168557-53-7/RN OR 2227-29-4/RN OR 40962-02-5/RN OR
                501419-30-3/RN OR 57-14-7/RN OR 627-19-0/RN OR 68928-07-4/RN
                OR 68928-08-5/RN OR 7087-68-5/RN OR 998-30-1/RN OR 100-42-5/RN
                OR 100-52-7/RN OR 10175-53-8/RN OR 1192-62-7/RN OR 123-72-8/RN
                OR 162157-02-0/RN OR 168557-47-9/RN OR
L46         12591 SEA FILE=CASREACT ABB=ON  PLU=ON  L45/PRO
L47            24 SEA FILE=CASREACT ABB=ON  PLU=ON  L29 (L) L46

=> s L47 not L60

L62            22 L47 NOT L60

=> file hcaplus

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FILE COVERS 1907 - 26 May 2006  VOL 144 ISS 23
FILE LAST UPDATED: 25 May 2006  (20060525/ED)

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 substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos L22

L5                STR
L6         428852 SEA FILE=REGISTRY SSS FUL L5
L7   (       7579)SEA FILE=REGISTRY ABB=ON  PLU=ON  IR>1
L8            725 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7/CAT
L9                STR
L11        424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
L13       2857503 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (RACT OR RCT OR RGT)/RL
L14               STR
L16          5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
L17          9286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16 (L) L13
L18            39 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L8
L19           837 SEA FILE=REGISTRY ABB=ON  PLU=ON  (12112-67-3/BI OR 617-86-7/BI
                  OR 1066-35-9/BI OR 107-05-1/BI OR 766-77-8/BI OR 10605-40-0/BI
```

```
                OR 18827-81-1/BI OR 603-35-0/BI OR 998-30-1/BI OR 29681-57-0/B
               I OR 7440-05-3/BI OR 7440-06-4/BI OR 111-78-4/BI OR 12246-51-4/
               BI OR 15243-33-1/BI OR 108-94-1/BI OR 12092-47-6/BI OR
               14694-95-2/BI OR 2031-62-1/BI OR 2487-90-3/BI OR 592-41-6/BI
               OR 7440-18-8/BI OR 789-25-3/BI OR 98-86-2/BI OR 100-42-5/BI OR
               100-52-7/BI OR 10210-68-1/BI OR 1079-66-9/BI OR 12111-11-4/BI
               OR 12148-71-9/BI OR 13938-94-8/BI OR 14857-34-2/BI OR 16941-92-
               7/BI OR 4342-22-7/BI OR 498-66-8/BI OR 536-74-3/BI OR 603-32-7/
               BI OR 64-17-5/BI OR 693-02-7/BI OR 7439-88-5/BI OR 7440-04-2/BI
                OR 776-76-1/BI OR 930-68-7/BI OR 10025-78-2/BI OR 10170-69-1/B
               I OR 1038-95-5/BI OR 104-53-0/BI OR 106-95-6/BI OR 1081-97-6/BI
                OR 109-89-7/BI OR 110-54-3/BI OR 1192-62-7/BI OR 12080-32-9/BI
                OR 12245-73-7/BI OR 123-72-8/BI OR 13269-52-8/BI OR 13829-48-6
               /BI OR 13829-50-0/BI OR 14221-01-3/BI OR 1438-82-0/BI OR
               1445-91-6/BI OR 146139-33-5/BI OR 14871-41-1/BI OR 148991-61-1/
               BI OR 14996-61-3/BI OR 1517-69-7/BI OR 15696-40-9/BI OR
               16941-12-1/BI OR 17685-52-8/BI OR 17718-70-6/BI OR 21693-13-0/B
               I OR 220800-76-0/BI OR 220800-77-1/BI OR 220800-78-2/BI OR
               220800-79-3/BI OR 24636-31-5/BI OR 2530-87-2/BI OR 25360-32-1/B
               I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
               /BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
               BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
               565-80-0/BI OR 583-60-8/BI OR 60255-04-1/BI OR 60255-25-6/BI
               OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
               OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
               656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
               I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
               75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/
L20          222 SEA FILE=REGISTRY ABB=ON  PLU=ON  L19 AND L11
L21         2871 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 (L) PREP/RL
L22           32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L21


=> d que nos L24

L5                STR
L6         428852 SEA FILE=REGISTRY SSS FUL L5
L7   (       7579)SEA FILE=REGISTRY ABB=ON  PLU=ON  IR>1
L8            725 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7/CAT
L9                STR
L11        424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
L13       2857503 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (RACT OR RCT OR RGT)/RL
L14               STR
L16          5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
L17          9286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16 (L) L13
L18            39 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L8
L19           837 SEA FILE=REGISTRY ABB=ON  PLU=ON  (12112-67-3/BI OR 617-86-7/BI
                  OR 1066-35-9/BI OR 107-05-1/BI OR 766-77-8/BI OR 10605-40-0/BI
                  OR 18827-81-1/BI OR 603-35-0/BI OR 998-30-1/BI OR 29681-57-0/B
                 I OR 7440-05-3/BI OR 7440-06-4/BI OR 111-78-4/BI OR 12246-51-4/
                 BI OR 15243-33-1/BI OR 108-94-1/BI OR 12092-47-6/BI OR
                 14694-95-2/BI OR 2031-62-1/BI OR 2487-90-3/BI OR 592-41-6/BI
                 OR 7440-18-8/BI OR 789-25-3/BI OR 98-86-2/BI OR 100-42-5/BI OR
                 100-52-7/BI OR 10210-68-1/BI OR 1079-66-9/BI OR 12111-11-4/BI
                 OR 12148-71-9/BI OR 13938-94-8/BI OR 14857-34-2/BI OR 16941-92-
                 7/BI OR 4342-22-7/BI OR 498-66-8/BI OR 536-74-3/BI OR 603-32-7/
                 BI OR 64-17-5/BI OR 693-02-7/BI OR 7439-88-5/BI OR 7440-04-2/BI
                  OR 776-76-1/BI OR 930-68-7/BI OR 10025-78-2/BI OR 10170-69-1/B
                 I OR 1038-95-5/BI OR 104-53-0/BI OR 106-95-6/BI OR 1081-97-6/BI
                  OR 109-89-7/BI OR 110-54-3/BI OR 1192-62-7/BI OR 12080-32-9/BI
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                OR 12245-73-7/BI OR 123-72-8/BI OR 13269-52-8/BI OR 13829-48-6
               /BI OR 13829-50-0/BI OR 14221-01-3/BI OR 1438-82-0/BI OR
               1445-91-6/BI OR 146139-33-5/BI OR 14871-41-1/BI OR 148991-61-1/
               BI OR 14996-61-3/BI OR 1517-69-7/BI OR 15696-40-9/BI OR
               16941-12-1/BI OR 17685-52-8/BI OR 17718-70-6/BI OR 21693-13-0/B
               I OR 220800-76-0/BI OR 220800-77-1/BI OR 220800-78-2/BI OR
               220800-79-3/BI OR 24636-31-5/BI OR 2530-87-2/BI OR 25360-32-1/B
               I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
               /BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
               BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
               565-80-0/BI OR 583-60-8/BI OR 60255-04-1/BI OR 60255-25-6/BI
               OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
               OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
               656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
               I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
               75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/
L20          222 SEA FILE=REGISTRY ABB=ON  PLU=ON  L19 AND L11
L21         2871 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 (L) PREP/RL
L22           32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L21
L23       405200 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (?ALKENE? OR ?DIENE?)/BI
L24           19 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L23

=> d que nos L26

L5                STR
L6         428852 SEA FILE=REGISTRY SSS FUL L5
L7   (       7579)SEA FILE=REGISTRY ABB=ON  PLU=ON  IR>1
L8            725 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7/CAT
L9                STR
L11        424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
L13       2857503 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (RACT OR RCT OR RGT)/RL
L14               STR
L16          5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
L17          9286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16 (L) L13
L18            39 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L8
L19           837 SEA FILE=REGISTRY ABB=ON  PLU=ON  (12112-67-3/BI OR 617-86-7/BI
                OR 1066-35-9/BI OR 107-05-1/BI OR 766-77-8/BI OR 10605-40-0/BI
                OR 18827-81-1/BI OR 603-35-0/BI OR 998-30-1/BI OR 29681-57-0/B
               I OR 7440-05-3/BI OR 7440-06-4/BI OR 111-78-4/BI OR 12246-51-4/
               BI OR 15243-33-1/BI OR 108-94-1/BI OR 12092-47-6/BI OR
               14694-95-2/BI OR 2031-62-1/BI OR 2487-90-3/BI OR 592-41-6/BI
               OR 7440-18-8/BI OR 789-25-3/BI OR 98-86-2/BI OR 100-42-5/BI OR
               100-52-7/BI OR 10210-68-1/BI OR 1079-66-9/BI OR 12111-11-4/BI
               OR 12148-71-9/BI OR 13938-94-8/BI OR 14857-34-2/BI OR 16941-92-
               7/BI OR 4342-22-7/BI OR 498-66-8/BI OR 536-74-3/BI OR 603-32-7/
               BI OR 64-17-5/BI OR 693-02-7/BI OR 7439-88-5/BI OR 7440-04-2/BI
                OR 776-76-1/BI OR 930-68-7/BI OR 10025-78-2/BI OR 10170-69-1/B
               I OR 1038-95-5/BI OR 104-53-0/BI OR 106-95-6/BI OR 1081-97-6/BI
                OR 109-89-7/BI OR 110-54-3/BI OR 1192-62-7/BI OR 12080-32-9/BI
                OR 12245-73-7/BI OR 123-72-8/BI OR 13269-52-8/BI OR 13829-48-6
               /BI OR 13829-50-0/BI OR 14221-01-3/BI OR 1438-82-0/BI OR
               1445-91-6/BI OR 146139-33-5/BI OR 14871-41-1/BI OR 148991-61-1/
               BI OR 14996-61-3/BI OR 1517-69-7/BI OR 15696-40-9/BI OR
               16941-12-1/BI OR 17685-52-8/BI OR 17718-70-6/BI OR 21693-13-0/B
               I OR 220800-76-0/BI OR 220800-77-1/BI OR 220800-78-2/BI OR
               220800-79-3/BI OR 24636-31-5/BI OR 2530-87-2/BI OR 25360-32-1/B
               I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
               /BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
               BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
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                565-80-0/BI OR 583-60-8/BI OR 60255-04-1/BI OR 60255-25-6/BI
                OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
                OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
                656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
                I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
                75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/
L20          222 SEA FILE=REGISTRY ABB=ON  PLU=ON  L19 AND L11
L21         2871 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 (L) PREP/RL
L22           32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L21
L25       793758 SEA FILE=HCAPLUS ABB=ON  PLU=ON  CONTINU?/BI
L26            2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L22 AND L25


=> d que nos L32

L4           7579 SEA FILE=REGISTRY ABB=ON  PLU=ON  IR>1
L5                STR
L6         428852 SEA FILE=REGISTRY SSS FUL L5
L9                STR
L11        424806 SEA FILE=REGISTRY SUB=L6 SSS FUL L9
L13       2857503 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (RACT OR RCT OR RGT)/RL
L14               STR
L16          5231 SEA FILE=REGISTRY SUB=L6 SSS FUL L14
L17          9286 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16 (L) L13
L19           837 SEA FILE=REGISTRY ABB=ON  PLU=ON  (12112-67-3/BI OR 617-86-7/BI
                  OR 1066-35-9/BI OR 107-05-1/BI OR 766-77-8/BI OR 10605-40-0/BI
                  OR 18827-81-1/BI OR 603-35-0/BI OR 998-30-1/BI OR 29681-57-0/B
                I OR 7440-05-3/BI OR 7440-06-4/BI OR 111-78-4/BI OR 12246-51-4/
                BI OR 15243-33-1/BI OR 108-94-1/BI OR 12092-47-6/BI OR
                14694-95-2/BI OR 2031-62-1/BI OR 2487-90-3/BI OR 592-41-6/BI
                OR 7440-18-8/BI OR 789-25-3/BI OR 98-86-2/BI OR 100-42-5/BI OR
                100-52-7/BI OR 10210-68-1/BI OR 1079-66-9/BI OR 12111-11-4/BI
                OR 12148-71-9/BI OR 13938-94-8/BI OR 14857-34-2/BI OR 16941-92-
                7/BI OR 4342-22-7/BI OR 498-66-8/BI OR 536-74-3/BI OR 603-32-7/
                BI OR 64-17-5/BI OR 693-02-7/BI OR 7439-88-5/BI OR 7440-04-2/BI
                  OR 776-76-1/BI OR 930-68-7/BI OR 10025-78-2/BI OR 10170-69-1/B
                I OR 1038-95-5/BI OR 104-53-0/BI OR 106-95-6/BI OR 1081-97-6/BI
                  OR 109-89-7/BI OR 110-54-3/BI OR 1192-62-7/BI OR 12080-32-9/BI
                  OR 12245-73-7/BI OR 123-72-8/BI OR 13269-52-8/BI OR 13829-48-6
                /BI OR 13829-50-0/BI OR 14221-01-3/BI OR 1438-82-0/BI OR
                1445-91-6/BI OR 146139-33-5/BI OR 14871-41-1/BI OR 148991-61-1/
                BI OR 14996-61-3/BI OR 1517-69-7/BI OR 15696-40-9/BI OR
                16941-12-1/BI OR 17685-52-8/BI OR 17718-70-6/BI OR 21693-13-0/B
                I OR 220800-76-0/BI OR 220800-77-1/BI OR 220800-78-2/BI OR
                220800-79-3/BI OR 24636-31-5/BI OR 2530-87-2/BI OR 25360-32-1/B
                I OR 28407-51-4/BI OR 4041-09-2/BI OR 4050-45-7/BI OR 4131-43-5
                /BI OR 4547-10-8/BI OR 502-42-1/BI OR 502-49-8/BI OR 5089-70-3/
                BI OR 51440-16-5/BI OR 51440-17-6/BI OR 563-80-4/BI OR
                565-80-0/BI OR 583-60-8/BI OR 60255-04-1/BI OR 60255-25-6/BI
                OR 60255-27-8/BI OR 603-36-1/BI OR 6163-58-2/BI OR 617-35-6/BI
                OR 62791-22-4/BI OR 65335-74-2/BI OR 656240-93-6/BI OR
                656240-94-7/BI OR 656240-95-8/BI OR 656240-96-9/BI OR 67-64-1/B
                I OR 74-85-1/BI OR 75-03-6/BI OR 75-64-9/BI OR 75-78-5/BI OR
                75-97-8/BI OR 7553-56-2/BI OR 75573-29-4/
L20          222 SEA FILE=REGISTRY ABB=ON  PLU=ON  L19 AND L11
L21         2871 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 (L) PREP/RL
L30         3438 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND X>0
L31          517 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 (L) CAT/RL
L32           23 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L31 AND L21
```

```
=> s (L22 or L24 or L26 or L32) not L59

L63          30 (L22 OR L24 OR L26 OR L32) NOT L59

=> dup rem L62 L63
FILE 'CASREACT' ENTERED AT 15:50:58 ON 26 MAY 2006
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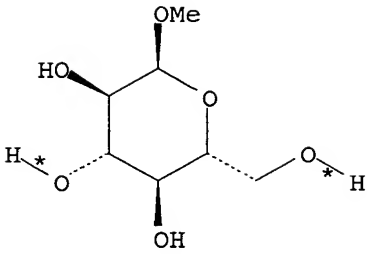
PROCESSING COMPLETED FOR L62
PROCESSING COMPLETED FOR L63
L64          38 DUP REM L62 L63 (14 DUPLICATES REMOVED)
                ANSWERS '1-22' FROM FILE CASREACT
                ANSWERS '23-38' FROM FILE HCAPLUS

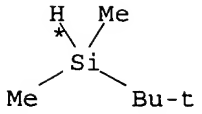
=> d ibib abs hit L64 1-22; d ibib abs hitind hitstr L64 23-38


L64  ANSWER 1 OF 38  CASREACT  COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         144:129167  CASREACT
TITLE:                    Regioselectively Trisilylated Hexopyranosides through
                          Homogeneously Catalyzed Silane Alcoholysis
AUTHOR(S):                Chung, Mee-Kyung; Schlaf, Marcel
CORPORATE SOURCE:         Guelph-Waterloo Centre for Graduate Work in Chemistry
                          (GWC), Department of Chemistry, University of Guelph,
                          Guelph, ON, N1G 2W1, Can.
SOURCE:                   Journal of the American Chemical Society (2005),
                          127(51), 18085-18092
                          CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   The iridium complex [Ir(COD)(PPh3)2]+SbF6- reacts with
     tert-butyldimethylsilane in DMA to form [IrH2(Sol)2(PPh3)2]+SbF6-, which
     is an active catalyst for the regioselective di- and trisilylation of a
     series of representative Me hexopyranosides, β-1,6-
     anhydrohexopyranosides and 1,3,5-O-methylidene inositol.  The
     corresponding 2,3,6- and 2,4,6-silylated glycosides are obtained in a
     separable mixture of 47-89% (2,3,6-isomers) and 9-25% (2,4,6-isomers) yield
     in a single-pot reaction.  The 2,4-disilylated derivs. of mannosan,
     galactosan, and 1,3,5-O-methylidene inositol as well as persilylated
     levoglucosan are accessible in >85% yield by this method.  The homogeneous
     nature of the catalysts is a prerequisite for the effective
     di-/trisilylation, as nanoparticle colloid catalysts generated in situ
     from Pd2(dba)3 (.apprx.1.5 nm average particle size) or Ru2Cl5(MeCN)7
     (.apprx.0.65 nm average particle size) result in only low yields.
REFERENCE COUNT:          28    THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


RX(5) OF 48     A  +  2 B  ===>  D
```

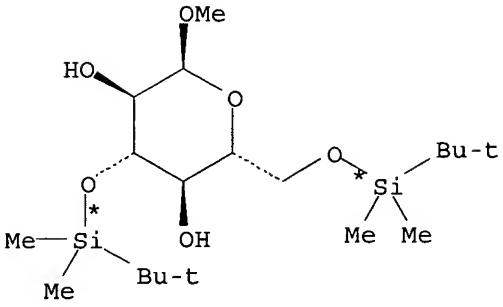


A



2 B

(5) →



D
YIELD 46%

RX(5) RCT A 97-30-3, B **29681-57-0**
PRO D **68102-62-5**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 127-19-5 AcNMe2
CON SUBSTAGE(1) 15 hours, room temperature
SUBSTAGE(2) 45 deg C
NTE other products also detected, regioselective

L64 ANSWER 2 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 142:56520 CASREACT
TITLE: Process for preparation of (haloalkyl)chlorosilanes by hydrosilylation of an alkenyl halide with a halosilane in presence of an iridium catalyst and an auxiliary ketone, ether, quinone, anhydride, unsatd. hydrocarbon or their mixtures
INVENTOR(S): Galland, Jean Christophe; Guennouni, Nathalie
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: Fr. Demande, 24 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

FR 2856402	A1	20041224	FR 2003-50222	20030617
FR 2856402	B1	20050826		
WO 2004113354	A2	20041229	WO 2004-FR1487	20040616
WO 2004113354	A3	20050317		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1633761	A2	20060315	EP 2004-767350	20040616

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

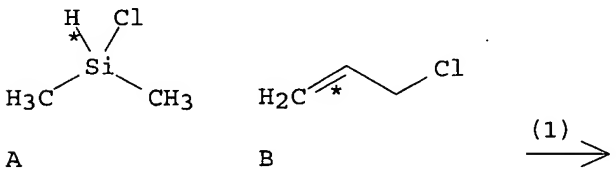
PRIORITY APPLN. INFO.: FR 2003-50222 20030617
WO 2004-FR1487 20040616

OTHER SOURCE(S): MARPAT 142:56520

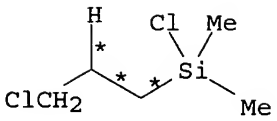
AB Dialkyl(halo)(haloalkyl)silanes XRR1Si(CH2)xX [X = Cl, Br, iodo; x = 2-10; R, R1 = (un)branched C1-6 alkyl, Ph] are prepared by hydrosilylation of an alkenyl halide CH2:CH(CH2)xX (same X, x) with a silane XRR2SiH (same X, R, R1) in presence of an Ir(I) or Ir(III) catalyst and an (un)supported auxiliary selected from the group of compds. including (i) ketones, (ii) ethers, (iii) quinones, (iv) anhydrides, (v) (a)cyclic C4-30 unsatd. hydrocarbons that are aromatic and/or contain at least one C:C double bond and/or at least one C.tplbond.C triple bond, where these unsatd. bonds may be conjugated, having 1-8 ethylene and/or acetylenic bonds and may have one or more heteroatoms, (vi) and their mixts., such that when the auxiliary is one or more unsatd. hydrocarbon, then this is combined with at least one other auxiliary of a different type. Preferably, ClSiMe2(CH2)3Cl is prepared from ClMe2SiH and allyl chloride in presence of [Ir(COD)Cl]2 and an auxiliary as defined above. In an example, treating 1.194 mol allyl chloride with 1.117 mol ClMe2SiH in presence of 2.829 x 10-5 mol [Ir(COD)Cl]2, 10.9 mmol cyclohexanone and 5.648 mmol COD for 2h 30 min at 20-25° and subsequent stirring for 20 min gave 98.3% ClSiMe2(CH2)3Cl.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 1 **A** + B ===> **C**



A B



C
YIELD 98%

RX(1) RCT A **1066-35-9**, B 107-05-1
PRO C **10605-40-0**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 108-94-1 Cyclohexanone, 111-78-4 1,5-COD
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 2.5 hours, 20 - 25 deg C
SUBSTAGE(3) 20 minutes, room temperature

L64 ANSWER 3 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 139:22334 CASREACT
TITLE: Method for obtaining bis(monoorganoxysilylpropyl) polysulfides
INVENTOR(S): Guennouni, Nathalie; Pevere, Virginie; Vogin, Bernard
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048169	A1	20030612	WO 2002-FR4204	20021206
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2833264	A1	20030613	FR 2001-15768	20011206
FR 2833264	B1	20050819		
FR 2833265	A1	20030613	FR 2002-10145	20020809
FR 2833265	B1	20060210		
AU 2002364429	A1	20030617	AU 2002-364429	20021206
EP 1461344	A1	20040929	EP 2002-799785	20021206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005511700	T2	20050428	JP 2003-549359	20021206
EP 1621543	A1	20060201	EP 2005-21616	20021206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR, BG, CZ, EE, SK				
PRIORITY APPLN. INFO.:			FR 2001-15768	20011206
			FR 2002-10145	20020809

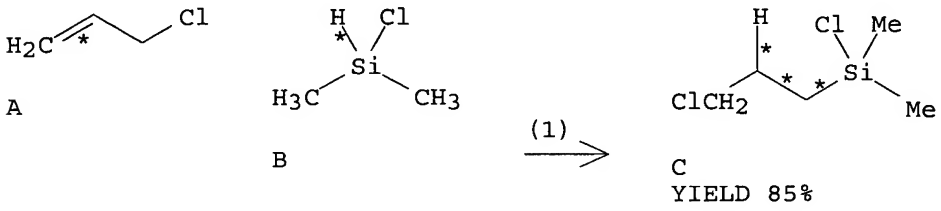
EP 2002-799785 20021206
WO 2002-FR4204 20021206

OTHER SOURCE(S): MARPAT 139:22334

AB The invention concerns the preparation of bis(monoorganooxysilylpropyl) polysulfides R1OSiR2R3(CH2)3-Sx-(CH2)3SiR2R3OR1 (I, R1 = C1-C15 alkyl, alkoxyalkyl; R2 and R3 = C1-C6 alkyl and/or phenyl; 1.5 ±.1 ≤ x ≤ 5 ±0.1). Said preparation is carried out by performing successively the following steps (a), (b) and (c): (a) hydrosilylation of the type: R2R3HSi-Hal + CH2:CH-CH2-Hal → Hal-R2R3Si-(CH2)3Hal; (b) alcoholysis of the type: Hal-R2R3Si-(CH2)3-Hal + R1OH → R1O-R2R3Si-(CH2)3Hal; (c) sulfidization of the type: R1O-R2R3Si-(CH2)3Hal + M2Sx → compound I; with Hal = halogen atom and M = alkali metal. Variations of the above reaction are also included in the invention. Thus, reaction of Me2HSiCl with CH2:CHCH2Cl in the presence of [Ir(COD)Cl]2 (COD = 1,5-cyclooctadiene) as catalyst afforded ClSiMe2(CH2)3Cl (85% yield), which reacted with ethanol to give EtOSiMe2(CH2)3Cl (96% yield). Finally, reaction of the latter with Na2S4 afforded bis(monoorganooxysilylpropyl) tetrasulfide, EtOSiMe2(CH2)3-S4-(CH2)3SiMe2OEt (87% yield).

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 6 A + **B** ===> **C**...



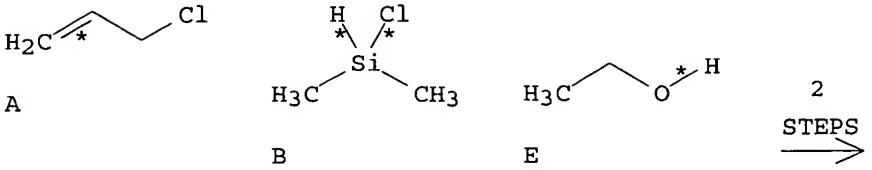
RX(1) RCT A 107-05-1

STAGE(1)
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
CON 20 deg C

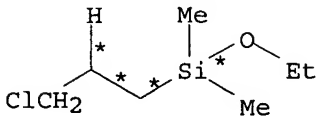
STAGE(2)
RCT B **1066-35-9**
CON SUBSTAGE(1) 155 minutes, 20 - 25 deg C
SUBSTAGE(2) 20 minutes, 20 - 25 deg C

PRO C **10605-40-0**
NTE key step

RX(4) OF 6 COMPOSED OF RX(1), RX(2)
RX(4) A + **B** + E ===> **F**



A B E 2 STEPS



F
YIELD 96%

RX(1) RCT A 107-05-1

STAGE(1)
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
CON 20 deg C

STAGE(2)
RCT B **1066-35-9**
CON SUBSTAGE(1) 155 minutes, 20 - 25 deg C
SUBSTAGE(2) 20 minutes, 20 - 25 deg C

PRO C 10605-40-0
NTE key step

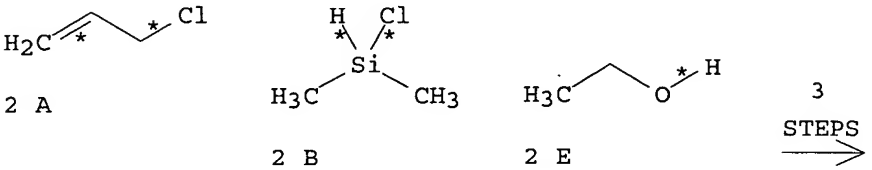
RX(2) RCT C 10605-40-0

STAGE(1)
CON 150 deg C, 1 atm

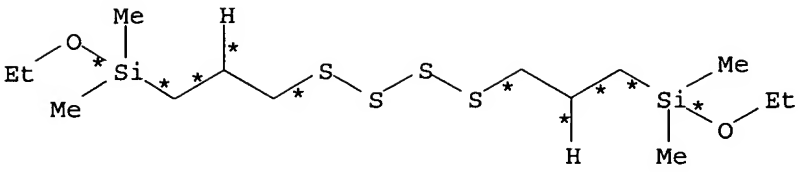
STAGE(2)
RCT E 64-17-5
CON 4.5 hours, 110 deg C, 1 atm

PRO F **13508-63-9**

RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)
RX(6) 2 A + 2 **B** + 2 E ===> **G**



2 A 2 B 2 E 3 STEPS



G
YIELD 87%

RX(1) RCT A 107-05-1

STAGE(1)
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
CON 20 deg C

STAGE(2)
RCT B **1066-35-9**
CON SUBSTAGE(1) 155 minutes, 20 - 25 deg C
SUBSTAGE(2) 20 minutes, 20 - 25 deg C

PRO C 10605-40-0
NTE key step

RX(2) RCT C 10605-40-0

STAGE(1)
CON 150 deg C, 1 atm

STAGE(2)
RCT E 64-17-5
CON 4.5 hours, 110 deg C, 1 atm

PRO F 13508-63-9

RX(3)

STAGE(1)
RGT H 12034-39-8 Sodium sulfide (Na2(S4))
SOL 64-17-5 EtOH
CON 80 deg C

STAGE(2)
RCT F 13508-63-9
CON SUBSTAGE(1) 80 deg C
SUBSTAGE(2) 2 hours, 80 deg C

PRO G **298689-48-2**

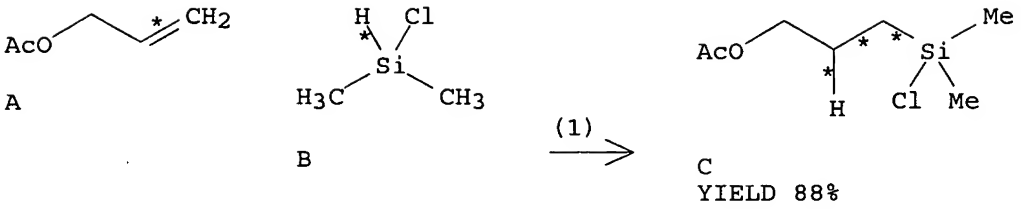
L64 ANSWER 4 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 138:287818 CASREACT
TITLE: Method for preparation of carboxylic acid 3-(dimethylchlorosilyl)propyl ester by hydrosilylation of carboxylic acid allyl ester with dimethylchlorosilane
INVENTOR(S): Nishiwaki, Hiromi; Kiyomori, Ayumu; Kubota, Toru;

Tonomura, Yoichi
PATENT ASSIGNEE(S): Shin-Etsu Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003096086	A2	20030403	JP 2001-296148	20010927

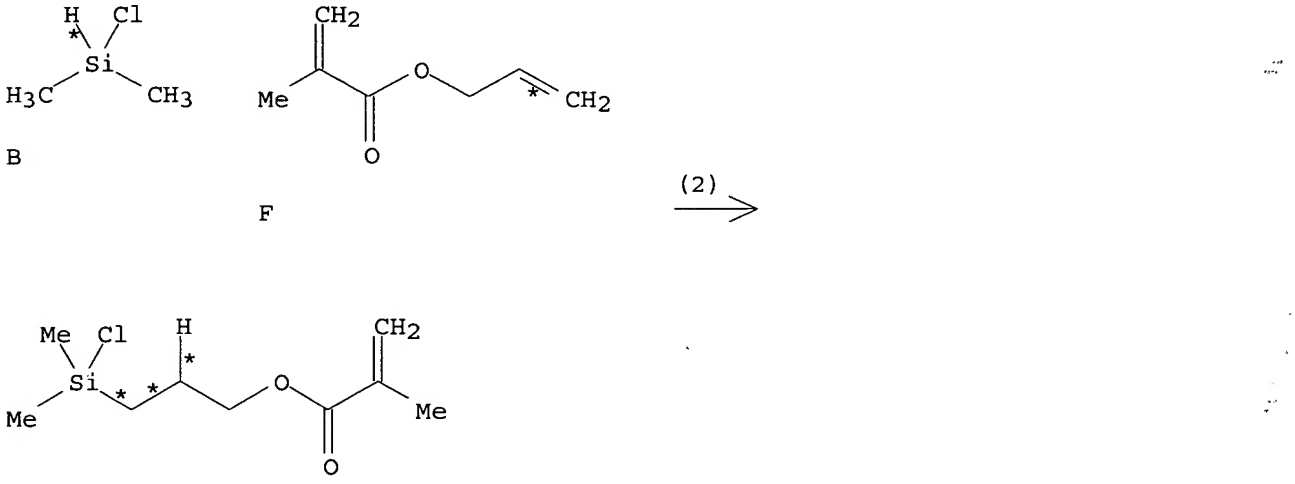
PRIORITY APPLN. INFO.: JP 2001-296148 20010927
OTHER SOURCE(S): MARPAT 138:287818
AB Carboxylic acid 3-(dimethylchlorosilyl)propyl esters represented by general formula RCO2(CH2)3SiMe3Cl (R = C1-10 monovalent hydrocarbon group) are prepared by hydrosilylation of a carboxylic acid allyl ester of formula RCO2CH2CH:CH2 (R = same as above) with dimethylchlorosilane in the presence of an iridium catalyst. The iridium catalyst is an iridium salt or an iridium complex represented by a general formula [Ir(R5)Y]3 (R5 = diene compound; Y = Cl, Br, iodo) and the hydrosilylation is carried out also in the presence of an ethylene derivative of formula R1R3C:CR2R4 (wherein R1 , R2 = C1-10 monovalent hydrocarbon group; or R1 and R2 are bonded to each other to form a C3-20 ring together with the carbon atom to which they are bonded; R3, R4 = H, C1-10 monovalent hydrocarbon group). This process sufficiently decreases the side reactions which presented problems in the past and gives in high yields the desired carboxylic acid 3-(dimethylchlorosilyl)propyl esters of high purity. The carboxylic acid 3-(dimethylchlorosilyl)propyl esters are widely used in industries as silane coupling agents, raw materials for modified silicon oils, and polymerizable monomers for silicon-containing polymers. Thus, allyl methacrylate 26.0, 2,6-di-tert-butyl-4-methylphenol (BHT) (polymerization inhibitor) 0.33, 1,5-cyclooctadiene 2.2, and di-μ-chlorobis(μ-1,5-cyclooctadiene)diiridium 0.017 g were added to a 4-neck 500 mL-flask equipped with a dropping funnel, a Dimroth condenser, a stirrer, and a thermometer and heated to 60° while passing N through an inlet of the condenser, followed by feeding dropwsie 94.6 g dimethylchlorosilane over 5.5 h while maintaining the reaction temperature at 60-65° by adjusting the dropping rate or through a heat medium, and the resulting mixture was aged at 60° for 0.4 5 h, cooled to room temperature to give 84.2% 3-(dimethylchlorosilyl)propyl methacrylate (I), 0.2% β-addition isomers, 0.2 methacryloxydimethylsilane, and 0.8% dimethyldichlorosilane as compared to 69.9% I, 2.4% β-adduct, 4.1% methacryloxydimethylsilane, and 2.4% dimethyldichlorosilane when chloroplatinic acid was used as the catalyst. The reaction mixture was distilled by a simple distillation apparatus to first distill volatile components at 38-48° (column top. temperature) and 2.4 KPa and then obtain 179.9 g of the main fraction containing 98.8% I and 0.2% β-adduct at 0.5 kPa (81.5 yield of I) and 48-85° (column top. temperature). Similarly, 3-(dimethylchlorosilyl)propyl acetate was obtained in 87.5% yield from allyl acetate and dimethyldichlorosilane.

RX(1) OF 2 A + **B** ===> **C**



RX(1) RCT A 591-87-7, B **1066-35-9**
PRO C **18387-98-9**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 111-78-4 1,5-COD
CON SUBSTAGE(1) 4 hours, 75 - 80 deg C
SUBSTAGE(2) 1 hour, 80 deg C
NTE hydrosilylation

RX(2) OF 2 **B** + F ===> **G**

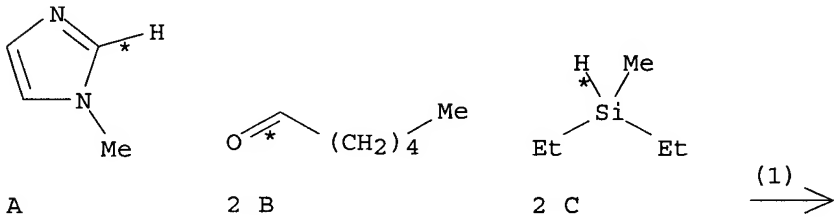


RX(2) RCT B **1066-35-9**, F 96-05-9
PRO G **24636-31-5**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 111-78-4 1,5-COD
CON SUBSTAGE(1) 5.5 hours, 60 - 65 deg C
SUBSTAGE(2) 0.5 hours, 60 deg C
NTE hydrosilylation

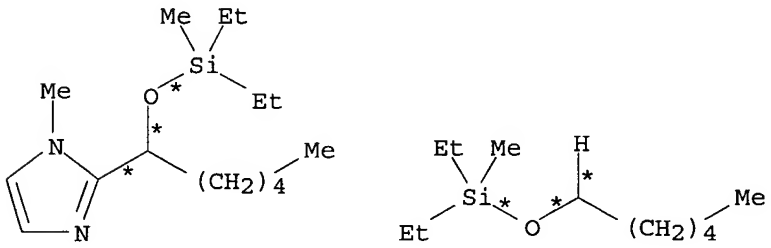
L64 ANSWER 5 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 138:55912 CASREACT
TITLE: [Ir4(CO)12]-catalyzed coupling reaction of imidazoles with aldehydes in the presence of a hydrosilane to give 2-substituted imidazoles

AUTHOR(S): Fukumoto, Yoshiya; Sawada, Katsutoshi; Hagihara, Motoyuki; Chatani, Naoto; Murai, Shinji
CORPORATE SOURCE: Department of Applied Chemistry Faculty of Engineering, Osaka University, Osaka, 565-0871, Japan
SOURCE: Angewandte Chemie, International Edition (2002), 41(15), 2779-2781
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A significant increase in yield is observed when DMAD is added to the reaction of 1-methylimidazole with aldehydes and diethylmethylsilane in the presence of a catalytic amount of [Ir4(CO)12] to produce 2-(1-diethylmethylsiloxyalkyl)imidazoles.
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 10 A + 2 B + 2 **C** ===> **D** + **E**



A 2 B 2 C

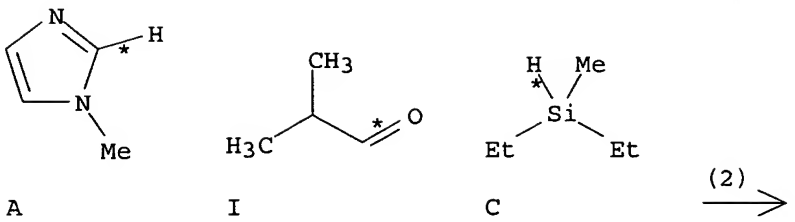


D
YIELD 92%(94)

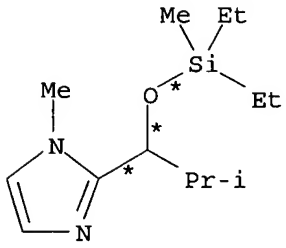
E
YIELD 92%(6)

RX(1) RCT A 616-47-7, B 66-25-1, C **760-32-7**
PRO D **479496-25-8**, E **479496-26-9**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 2 hours, reflux
SUBSTAGE(4) reflux -> room temperature

RX(2) OF 10 A + I + **C** ===> **J**



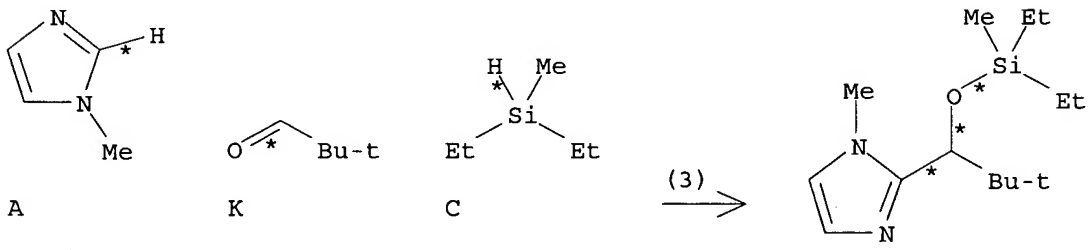
A I C (2)



J
YIELD 91%

RX(2) RCT A 616-47-7, I 78-84-2, C **760-32-7**
PRO J **479496-27-0**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 3 hours, reflux
SUBSTAGE(4) reflux -> room temperature

RX(3) OF 10 A + K + **C** ===> **L**



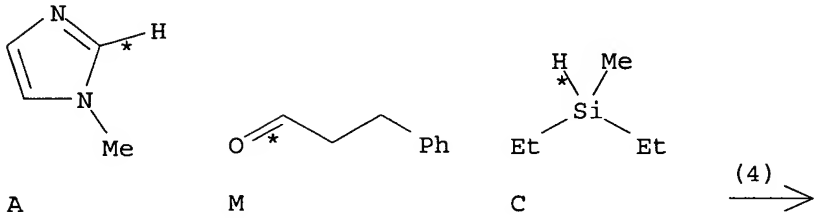
A K C (3)

L
YIELD 76%

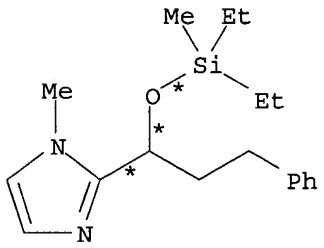
RX(3) RCT A 616-47-7, K 630-19-3, C **760-32-7**
PRO L **479496-28-1**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro,

762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 4 hours, reflux
SUBSTAGE(4) reflux -> room temperature

RX(4) OF 10 A + M + **C** ===> **N**



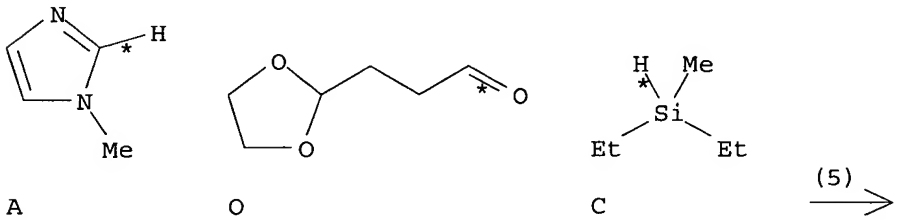
A M C



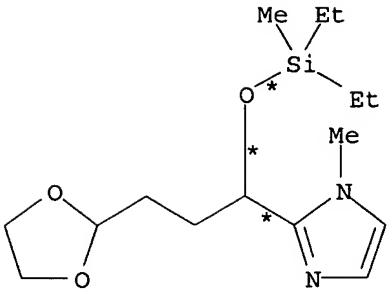
N
YIELD 72%

RX(4) RCT A 616-47-7, M 104-53-0, C **760-32-7**
PRO N **479496-29-2**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro,
762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 1 hour, reflux
SUBSTAGE(4) reflux -> room temperature

RX(5) OF 10 A + O + **C** ===> **P**



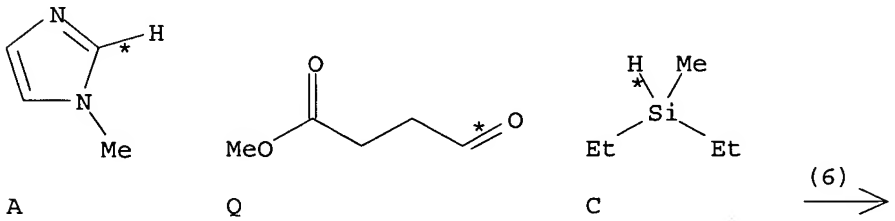
A O C



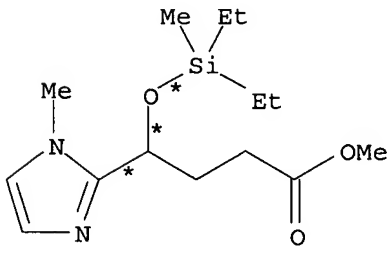
P
YIELD 62%

RX(5) RCT A 616-47-7, O 82962-18-3, C **760-32-7**
PRO P **479496-30-5**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 1 hour, reflux
SUBSTAGE(4) reflux -> room temperature

RX(6) OF 10 A + Q + **C** ===> **R**



A Q C (6)

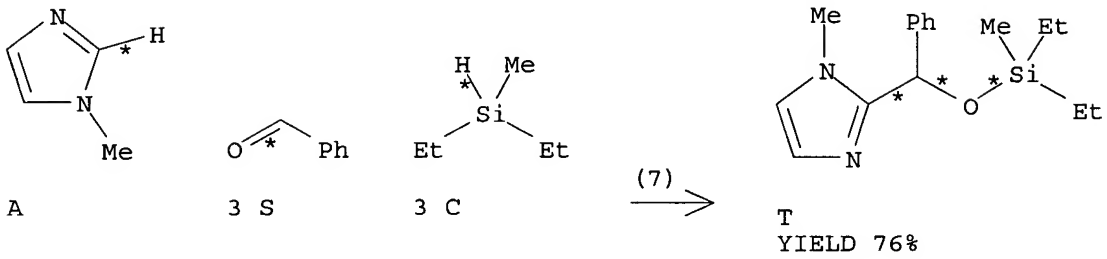


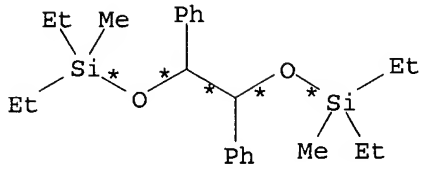
R
YIELD 87%

RX(6) RCT A 616-47-7, Q 13865-19-5, C **760-32-7**
PRO R **479496-31-6**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro,

762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 1 hour, reflux
SUBSTAGE(4) reflux -> room temperature

RX(7) OF 10 A + 3 S + 3 **C** ===> **T** + **U**

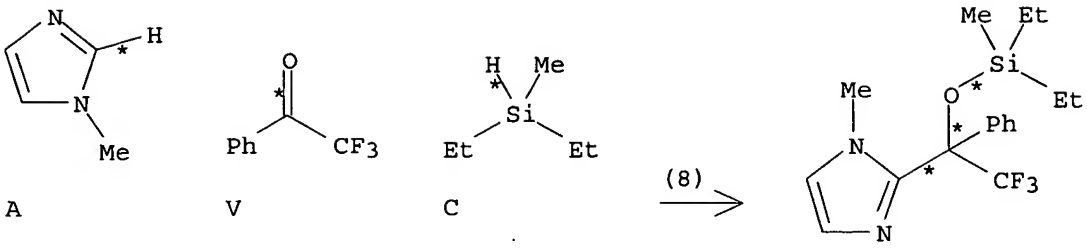




U
YIELD 8%

RX(7) RCT A 616-47-7, S 100-52-7, C **760-32-7**
PRO T **479496-32-7**, U **96206-22-3**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro,
762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 2 hours, reflux
SUBSTAGE(4) reflux -> room temperature

RX(8) OF 10 A + V + **C** ===> **W**

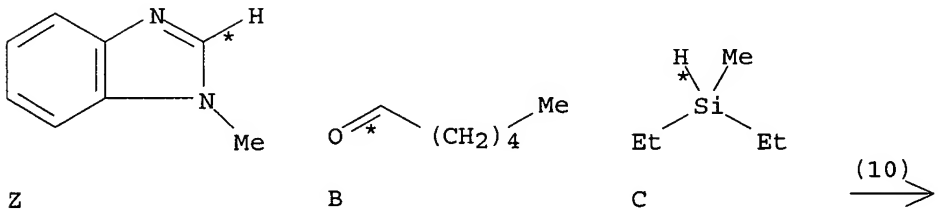


A V C (8) W

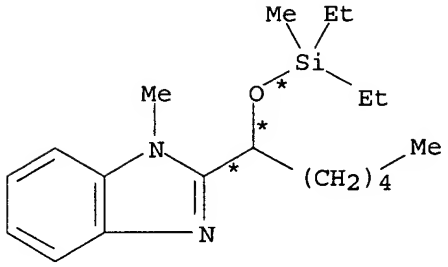
YIELD 32%

RX(8) RCT A 616-47-7, V 434-45-7, C **760-32-7**
PRO W **479496-33-8**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 762-42-5 DMADC
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 3 hours, reflux
SUBSTAGE(4) reflux -> room temperature

RX(10) OF 10 Z + B + **C** ===> **AA**



Z B C (10)



AA
YIELD 58%

RX(10) RCT Z 1632-83-3, B 66-25-1, C **760-32-7**
PRO AA **479496-35-0**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 762-42-5 DMADC

SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> reflux
SUBSTAGE(3) 19 hours, reflux
SUBSTAGE(4) reflux -> room temperature

L64 ANSWER 6 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 135:371860 CASREACT
TITLE: Preparation of halopropyldimethylchlorosilanes
INVENTOR(S): Tonomura, Yoichi; Kubota, Toru; Endo, Mikio
PATENT ASSIGNEE(S): Shin-Etsu Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

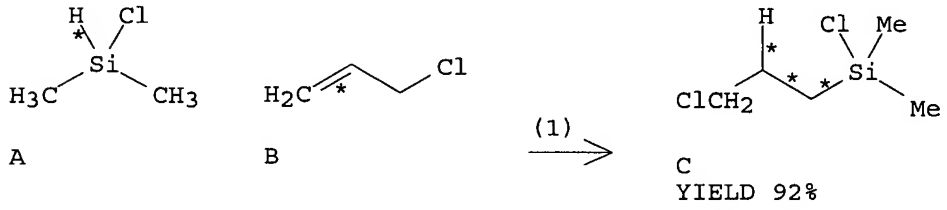
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001322993	A2	20011120	JP 2000-142128	20000515
US 2001053861	A1	20011220	US 2001-852638	20010511
US 6359161	B2	20020319		
EP 1156052	A2	20011121	EP 2001-304327	20010515
EP 1156052	A3	20030917		
EP 1156052	B1	20060208		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

PRIORITY APPLN. INFO.: JP 2000-142128 20000515
OTHER SOURCE(S): MARPAT 135:371860

AB The compds. XCH2CH2CH2SiMe2Cl (X = Cl, Br, I) are prepd by reaction of Me2SiHCl with XCH2CH:CH2 (X = same as above) in the presence of Ir catalysts and R1CR3C:CR2R4 (R1, R2 = C1-10 hydrocarbyl; R1R2 may form ring; R3, R4 = H, C1-10 hydrocarbyl). Me2SiHCl was reacted with allyl chloride in the presence of di-μ-chlorobis(μ-1,5-cyclooctadiene)diiridium and 1,5-cyclooctadiene at 35-40° for 7 h to give 92.7% 3-chloropropyldimethylchlorosilane.

RX(1) OF 1 **A** + B ===> **C**



A B C
YIELD 92%

RX(1) RCT A **1066-35-9**, B 107-05-1
PRO C **10605-40-0**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 111-78-4 1,5-COD

L64 ANSWER 7 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 131:116373 CASREACT

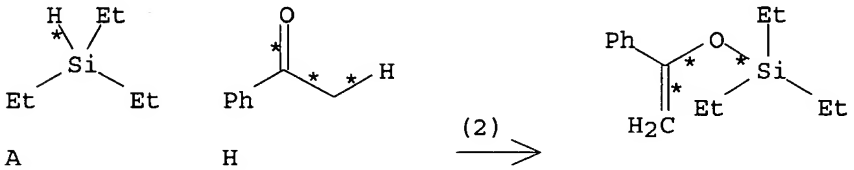
TITLE: Preparation of silyl enol ethers
INVENTOR(S): Fuchigami, Takamasa; Igarashi, Yasushi
PATENT ASSIGNEE(S): Sagami Chemical Research Center, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11217391	A2	19990810	JP 1998-15904	19980128

PRIORITY APPLN. INFO.: JP 1998-15904 19980128
OTHER SOURCE(S): MARPAT 131:116373

AB Title compds. RC(OSiR1R2R3):CR4R5 (R, R1, R2, R3, R4, R5 = H, alkyl, aryl, etc.) were prepared by reaction of ketones RCOCHR4R5 with HSiR1R2R3 in the presence of group 7-10 metals, halides, and amines. Thus, reaction of cyclohexanone with Et3SiH in toluene in the presence of 5% Pd/C, EtI, and Et3N at 100° for 16 h gave 87.1% 1-triethylsiloxycyclohexene.

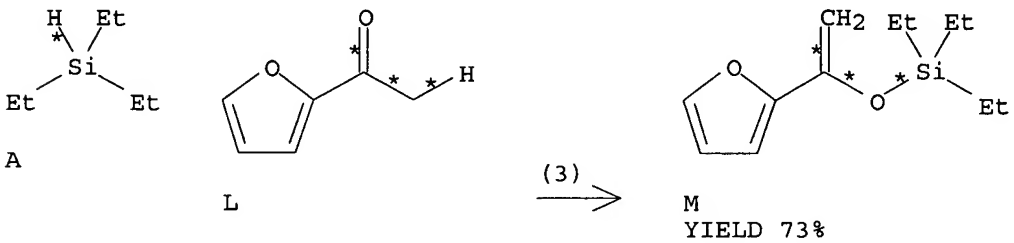
RX(2) OF 3 **A** + H ===> **I**



YIELD 74%

RX(2) RCT A **617-86-7**, H 98-86-2
PRO I **17718-70-6**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 75-03-6 EtI, 109-89-7 Et2NH
SOL 108-88-3 PhMe

RX(3) OF 3 **A** + L ===> **M**



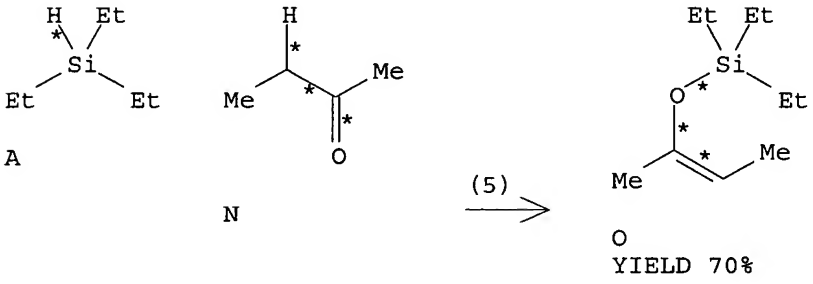
YIELD 73%

RX(3) RCT A **617-86-7**, L 1192-62-7
PRO M **220800-79-3**

CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro,
75-03-6 EtI, 109-89-7 Et2NH
SOL 108-88-3 PhMe

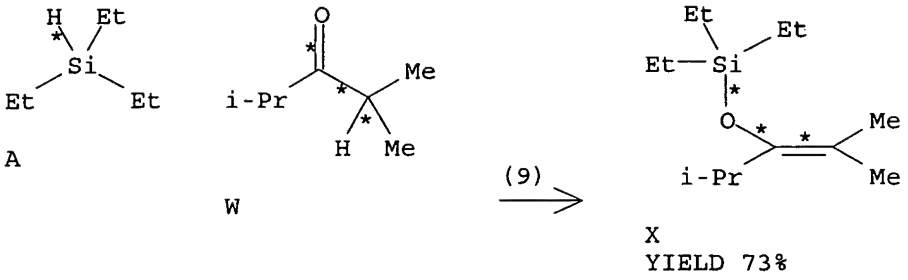
L64 ANSWER 8 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 8
ACCESSION NUMBER: 130:196694 CASREACT
TITLE: Transition metal-catalyzed dehydrogenative silylation of ketones with amine and halide as cocatalysts
AUTHOR(S): Igarashi, Mamoru; Sugihara, Yuichi; Fuchikami, Takamasa
CORPORATE SOURCE: Sagami Chemical Research Center, Kanagawa, 229-0012, Japan
SOURCE: Tetrahedron Letters (1999), 40(4), 711-714
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Dehydrogenative silylation of ketones with hydrosilanes proceeds in the presence of a transition metal catalyst such as Pd on C or Ir carbonyl, with amine and halide as cocatalysts, to give the corresponding silyl enol ethers in good yields. The present reaction is applicable for a variety of ketones and hydrosilanes with complete regioselectivity.
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 11 **A** + N ===> **O**



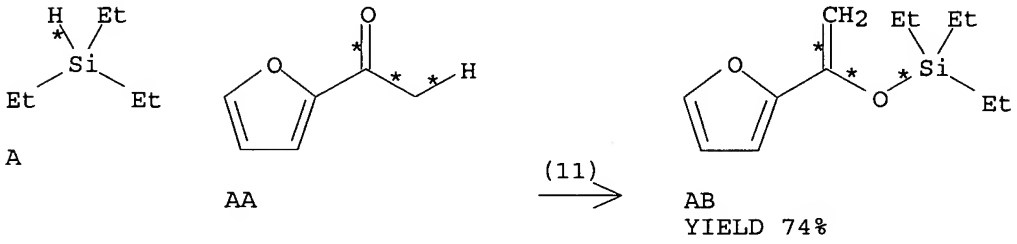
RX(5) RCT A **617-86-7**, N 78-93-3
PRO O **13829-50-0**
CAT 109-89-7 Et2NH, 75-03-6 EtI, **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 108-88-3 PhMe
NTE regioselective

RX(9) OF 11 **A** + W ===> **X**



RX(9) RCT A **617-86-7**, W 565-80-0
PRO X **80239-20-9**
CAT 109-89-7 Et2NH, 75-03-6 EtI, **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 108-88-3 PhMe
NTE regioselective

RX(11) OF 11 **A** + AA ===> **AB**



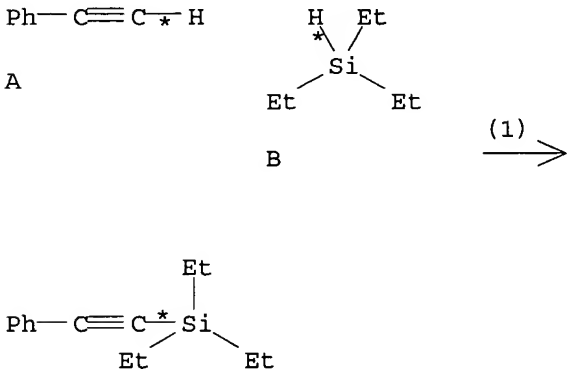
RX(11) RCT A **617-86-7**, AA 1192-62-7
PRO AB **220800-79-3**
CAT 109-89-7 Et2NH, 75-03-6 EtI, **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 108-88-3 PhMe
NTE regioselective

L64 ANSWER 9 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 127:358956 CASREACT
TITLE: Process for preparation of alkynylsilianes by catalytic coupling reaction
INVENTOR(S): Fuchigami, Takamasa; Shimizu, Rie
PATENT ASSIGNEE(S): Zaidan Hojin Sagami Chemical Research Center, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 09295986 A2 19971118 JP 1996-340782 19961220
PRIORITY APPLN. INFO.: JP 1996-51350 19960308
OTHER SOURCE(S): MARPAT 127:358956
AB The title compds. R'C.tplbond.CSiR3 (I; R = alkyl, alkenyl, aryl, etc.; R' = H, alkyl, alkenyl, aryl, etc.), are prepared by reacting HSiR3 with R'C.tplbond.CH (II; R' = same as above) in the presence of iridium carbonyl catalysts. I, useful materials in organic synthesis, are prepared in high yield easily. Thus, II (R' = Ph) was reacted with HSiEt3 in the presence of Ir4(CO)12 at 100° for 24 h to give 96% I (R = Et, R' = Ph).

RX(1) OF 1 A + **B** ===> **C**



A

B

C

YIELD 96%

RX(1) RCT A 536-74-3, B **617-86-7**
PRO C **4131-43-5**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro, 603-35-0 PPh3
SOL 110-71-4 (CH2OMe)2
NTE 100° for 24 h

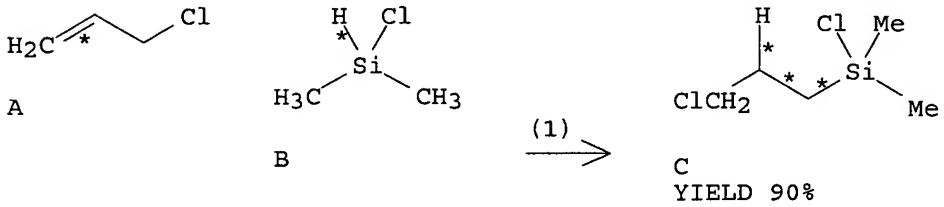
L64 ANSWER 10 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 10
ACCESSION NUMBER: 123:340390 CASREACT
TITLE: Preparation of (halopropyl)dimethylchlorosilane and catalysts used in the preparation
INVENTOR(S): Kubota, Tooru; Yamamoto, Akira; Endo, Mikio
PATENT ASSIGNEE(S): Shinetsu Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07126271	A2	19950516	JP 1993-270278	19931028
JP 2938731	B2	19990825		

PRIORITY APPLN. INFO.: JP 1993-270278 19931028
OTHER SOURCE(S): MARPAT 123:340390

AB (Halopropyl)dimethylchlorosilane, useful as an intermediate for silane coupling agents and as a modifier for silicone oils (no data), is prepared by treatment of Me2SiHCl with XCH2CH:CH2 (X = Cl, Br, I) in the presence of [IrRY]2 (R = diene; Y = Cl, Br, I). Me2SiHCl was added dropwise to a mixture of allyl chloride and di-μ-chlorobis(η4-1,5-cyclooctadiene)diiridium at 35-40° over 1 h and left at 40° for 1 h to give 90.5% (3-chloropropyl)dimethylchlorosilane.

RX(1) OF 1 A + **B** ===> **C**

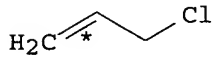


RX(1) RCT A 107-05-1, B **1066-35-9**
PRO C **10605-40-0**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-

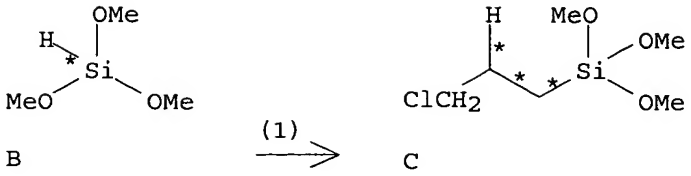
L64 ANSWER 11 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 11
ACCESSION NUMBER: 119:180892 CASREACT
TITLE: Ruthenium complex-catalyzed hydrosilylation of allyl chloride with trimethoxysilane
AUTHOR(S): Tanaka, Masato; Hayashi, Teruyuki; Mi, Zhi Yuan
CORPORATE SOURCE: Natl. Chem. Lab. Ind., Tsukuba, 305, Japan
SOURCE: Journal of Molecular Catalysis (1993), 81(2), 207-14
CODEN: JMCADS; ISSN: 0304-5102
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The hydrosilylation of allyl chloride with trimethoxysilane has been examined in the presence of several homogeneous complex catalysts. Iridium and ruthenium complexes exhibit higher selectivities in the reaction to give (3-chloropropyl)trimethoxysilane. Other complexes usually give propylene and/or tetramethoxysilane as side products in large quantities. The Ru3(CO)12-catalyzed reactions effected at lower temps. or by using a large excess of trimethoxysilane relative to allyl chloride give the chloropropylsilane in good yields.

RX(1) OF 2 A + **B** ===> **C**



A



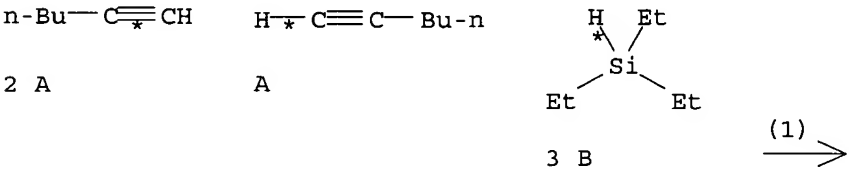
B C

RX(1) RCT A 107-05-1, B **2487-90-3**
PRO C **2530-87-2**
CAT **12246-51-4** Cyclooctene Ir
SOL 108-88-3 PhMe
NTE other products also formed

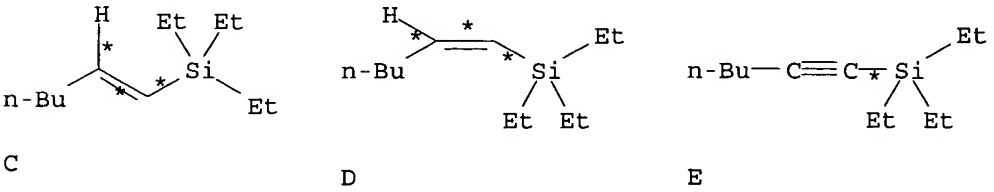
L64 ANSWER 12 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 12
ACCESSION NUMBER: 110:24071 CASREACT
TITLE: Iridium catalyzed hydrosilylation of 1-hexyne: the unusual formation of 1-(triethylsilyl)-1-hexyne
AUTHOR(S): Fernandez, Maria J.; Oro, Luis A.; Manzano, Blanca R.
CORPORATE SOURCE: Inst. Cienc. Mater. Aragon, Univ. Zaragoza, Zaragoza, 50009, Spain
SOURCE: Journal of Molecular Catalysis (1988), 45(1), 7-15
CODEN: JMCADS; ISSN: 0304-5102
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 1-Hexyne undergoes reaction with Et3SiH in the presence of IrH2(SiEt3)(COD)(AsPh3) (COD = 1,5-cyclooctadiene) or Ir catalysts formed by adding triarylarsines or triarylphosphines to [Ir(OMe)(diolefin)]2. The products of the catalytic reaction are the expected trans- and cis-1-triethylsilylhex-1-enes, as well as significant amts. of 1-triethylsilylhex-1-yne and 1-hexene. Mechanistic pathways for the observed hydrosilylation reaction are discussed, including the possible participation of a vinylidene-iridium intermediate formed from hydridoalkynyliridium species.

RX(1) OF 7 3 A + 3 **B** ===> **C** + **D** + **E**



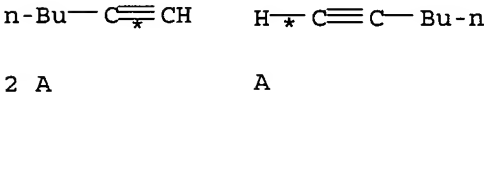
2 A A 3 B



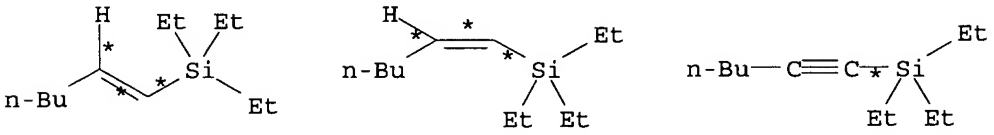
C D E

RX(1) RCT A 693-02-7, B **617-86-7**
PRO C **42067-72-1**, D **62621-38-9**, E **21693-13-0**
CAT **94401-81-7** Iridium, di-μ-methoxybis[(2,3,9,10-η)-5,6,7,8-tetrafluoro-1,4-dihydro-1,4-ethenonaphthalene]di-
SOL 107-06-2 ClCH2CH2Cl
NTE Reaction was also carried out in presence of phosphines or arsines

RX(2) OF 7 3 A + 3 **B** ===> **C** + **D** + **E**



2 A A 3 B



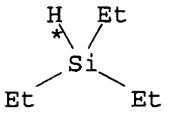
C D E

RX(2) RCT A 693-02-7, B **617-86-7**
PRO C **42067-72-1**, D **62621-38-9**, E **21693-13-0**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-
SOL 107-06-2 ClCH2CH2Cl
NTE Reaction was also carried out in presence of phosphines or arsines

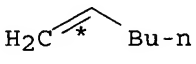
L64 ANSWER 13 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 13
ACCESSION NUMBER: 107:59087 CASREACT
TITLE: Hydrosilylation of alkenes by iridium complexes
AUTHOR(S): Oro, L. A.; Fernandez, M. J.; Esteruelas, M. A.; Jimenez, M. S.
CORPORATE SOURCE: Inst. Cienc. Mater. Aragon., Univ. Zaragoza, Saragossa, 50009, Spain
SOURCE: Journal of Molecular Catalysis (1986), 37(2-3), 151-6
CODEN: JMCADS; ISSN: 0304-5102
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [IrX(COD)]2 (X = OMe, Cl; COD = cyclooctadiene) with monodentate Group Vb atom donor ligands (NPh3, PPh3, AsPh3, SbPh3) yielded a mixture of hexenyltriethylsilanes as well as the expected hexyltriethylsilane from the catalytic hydrosilylation of hex-1-ene by Et3SiH. The most effective catalysts are those derived from [IrCl(COD)]2 + 2 PPh3 + 2 AsPh3 and

[Ir(OMe)(COD)]2 + 2 AsPh3. The latter system was active for hydrosilylation reactions involving ethylene and propylene. The catalyst systems studied include [IrX(COD)]2 + 2L (X = OMe, L = NPh3, PPh3, AsPh3, SbPh3; X = Cl, L = PPh3, AsPh3), [Ir(OMe)(COD)]2 + 4L (L = PPh3, AsPh3) and [IrX(COD)]2 + 2PPh3 + 2AsPh3 (X = OMe, Cl).

RX(1) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**...

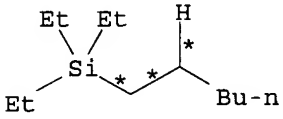


2 A

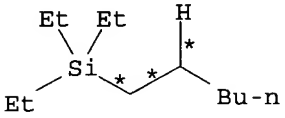


3 B

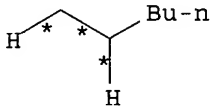
(1)



C: CM 1



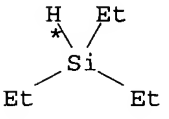
D



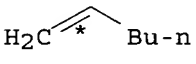
E

RX(1) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-34-9 Benzenamine, N,N-diphenyl-
SOL 107-06-2 ClCH2CH2Cl

RX(2) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**

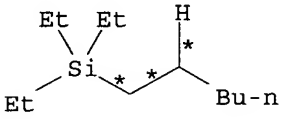


2 A

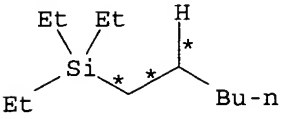


3 B

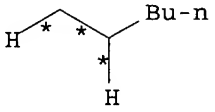
(2)



C: CM 1



D

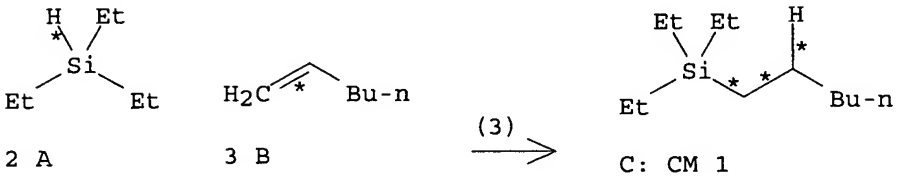


E

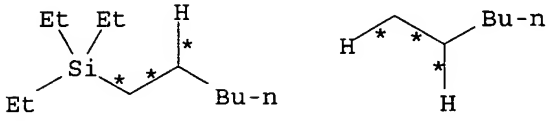
RX(2) RCT A **617-86-7**, B 592-41-6

PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-35-0 PPh3
SOL 107-06-2 ClCH2CH2Cl

RX(3) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**



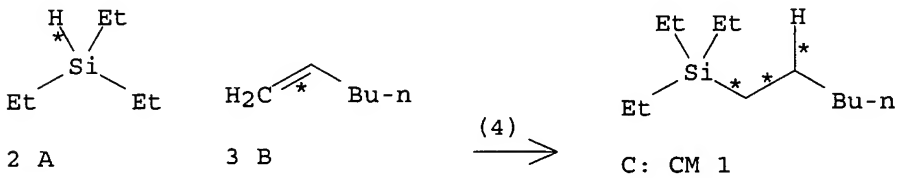
2 A 3 B C: CM 1



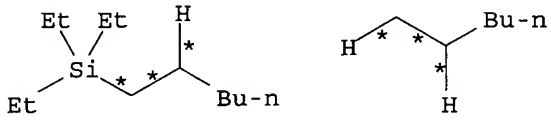
D E

RX(3) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-32-7 Ph3As
SOL 107-06-2 ClCH2CH2Cl

RX(4) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**



2 A 3 B C: CM 1

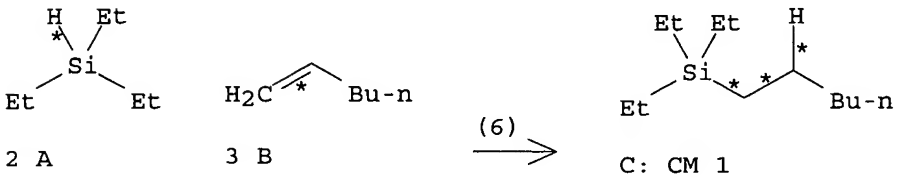


D E

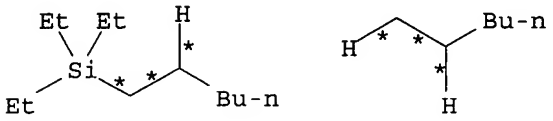
RX(4) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**

CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-36-1 Ph3Sb
SOL 107-06-2 ClCH2CH2Cl

RX(6) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**



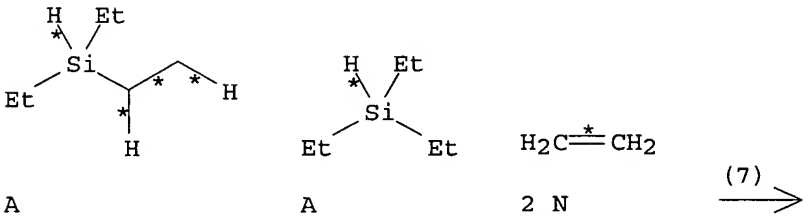
2 A 3 B (6) C: CM 1



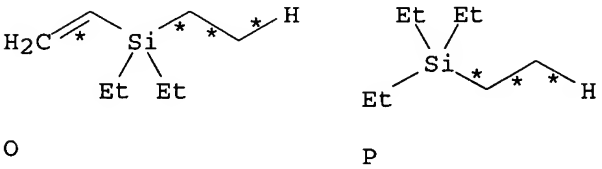
D E

RX(6) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 603-32-7 Ph3As
SOL 107-06-2 ClCH2CH2Cl

RX(7) OF 14 2 **A** + 2 N ===> **O** + **P**



A A 2 N (7)

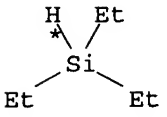


O P

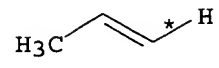
RX(7) RCT A **617-86-7**, N 74-85-1
PRO O **1112-54-5**, P **631-36-7**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-32-7 Ph3As

SOL 75-09-2 CH2Cl2

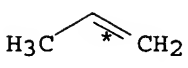
RX(8) OF 14 2 **A** + 2 R ===> **S** + **T**



2 A

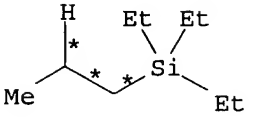


R

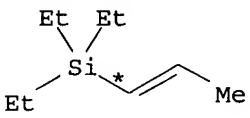


R

(8)



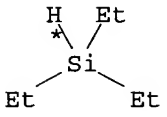
S



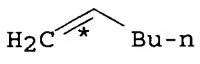
T

RX(8) RCT A **617-86-7**, R 115-07-1
PRO S **994-44-5**, T **3931-84-8**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-32-7 Ph3As
SOL 75-09-2 CH2Cl2

RX(9) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**

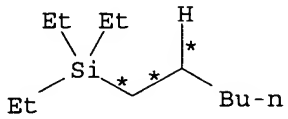


2 A

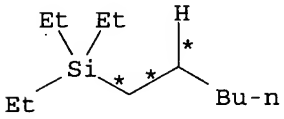


3 B

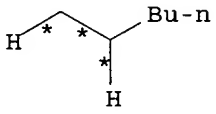
(9)



C: CM 1



D

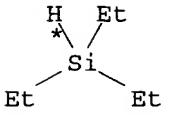


E

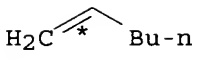
RX(9) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-35-0 PPh3, 603-32-7 Ph3As
SOL 107-06-2 ClCH2CH2Cl

RX(10) OF 14 2 **A** + 3 B ===> **C** + **D** +

E

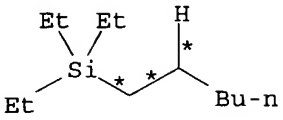


2 A



3 B

(10)



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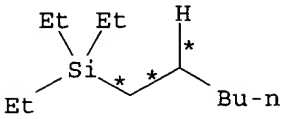
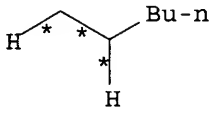


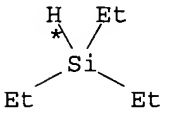
D



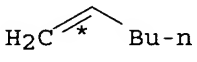
E

RX(10) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 603-35-0 PPh3, 603-32-7 Ph3As
SOL 107-06-2 ClCH2CH2Cl

RX(11) OF 14 2 **A** + 3 B ===> **C** + **D** + **E**

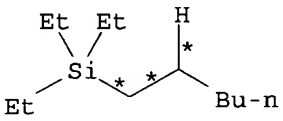


2 A

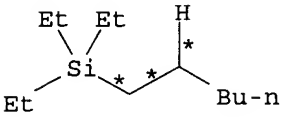


3 B

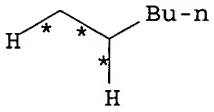
(11)



C: CM 1



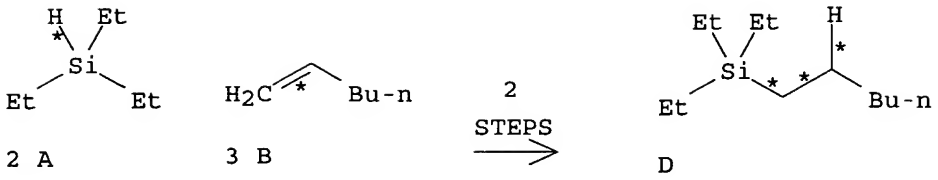
D



E

RX(11) RCT A **617-86-7**, B 592-41-6
PRO C **109389-69-7**, D **13810-04-3**, E **110-54-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 603-35-0 PPh3
SOL 107-06-2 ClCH2CH2Cl

RX(14) OF 14 COMPOSED OF RX(1), RX(13)
RX(14) 2 **A** + 3 B ===> **D**

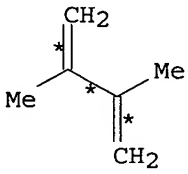


RX(1) RCT A **617-86-7**, B 592-41-6
PRO C 109389-69-7, D **13810-04-3**, E 110-54-3
CAT **12148-71-9** Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-, 603-34-9 Benzenamine, N,N-diphenyl-
SOL 107-06-2 ClCH2CH2Cl

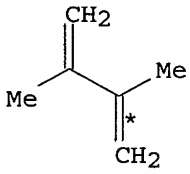
RX(13) RCT C 109389-69-7
RGT Y 1333-74-0 H2
PRO D **13810-04-3**
CAT 52657-94-0 Iridium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene]bis(triphenylphosphine)-, perchlorate

L64 ANSWER 14 OF 38 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 14
ACCESSION NUMBER: 103:178404 CASREACT
TITLE: Iridium complexes as hydrosilylation catalysts
AUTHOR(S): Apple, David C.; Brady, Karen A.; Chance, Jeffrey M.; Heard, Nina E.; Nile, Terence A.
CORPORATE SOURCE: Dep. Chem., Univ. North Carolina, Greensboro, NC, 27412, USA
SOURCE: Journal of Molecular Catalysis (1985), 29(1), 55-64
CODEN: JMCADS; ISSN: 0304-5102
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [IrClL2]2 (I; L = cyclooctene) (II) catalyzed hydrosilylation of H2C:CMeCMe:CH2, giving predominantly the 1,4 adducts Me2CC:CMeCH2SiR3 (R = Et, OEt); addition of PPh3 decreased the yield. Hydrosilylation of PrC.tplbond.CH with HSiEt3 using II or II-PR13 (R1 = Ph, C6H4Me-2) gave 62-100% PrCH:CHSiEt3 containing 70-83% of the cis isomer. Hydrosilylation of cyclohexanone, in 64-75% yield, was also catalyzed by II or II-PPh3 but addition of 2 equiv PPh3 gave the catalytically inert IrHCl(SiEt3)(PPh3)2. Hydrosilylation of 1-octene using II or II-PR13 (same R1) proceeded in only 4-30% yield to 1-octylsilanes. Hydrosilylation of 2-cyclohexenone with HSiEt3 using I (L = 1,5-cyclooctadiene) (III) or II occurred largely by 1,2-addition to give 2-cyclohexenol in 69-76% selectively following hydrolysis. Replacing HSiEt3 with H2SiMePh gave only 2-cyclohexenol. However, using II-PPh3 increased the formation of 1,4-addition product in both cases. Attempted asym. induction using MeCOCO2Et or PhAc, III, H2SiPh2, and chiral diphosphines gave 0-7% enantiomeric excesses.

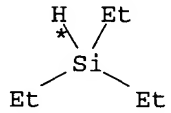
RX(1) OF 43 2 A + 2 **B** ===> **C** + **D**



A

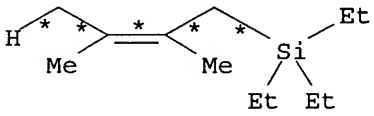


A

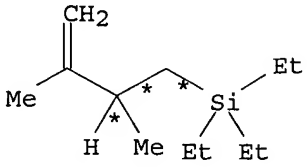


2 B

(1) →



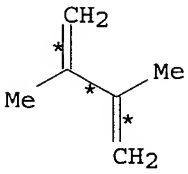
C



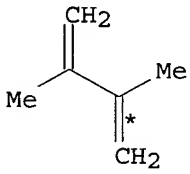
D

RX(1) RCT A 513-81-5, B **617-86-7**
PRO C **64545-12-6**, D **64578-20-7**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat. The 1, 4-adduct was the major product

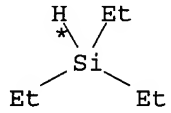
RX(2) OF 43 2 A + 2 **B** ===> **C** + **D**



A

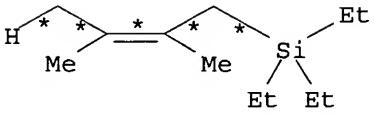


A

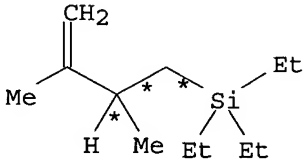


2 B

(2) →



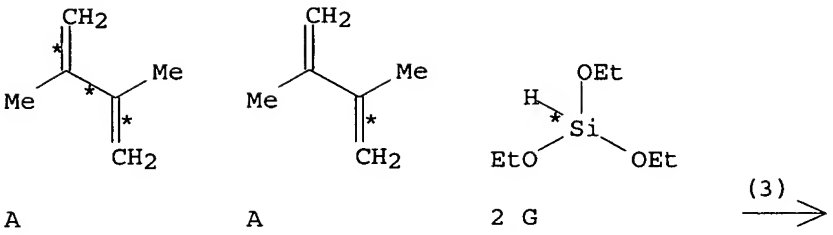
C



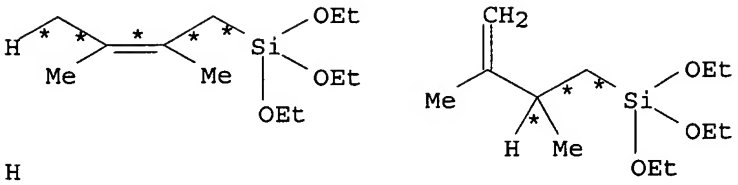
D

RX(2) RCT A 513-81-5, B **617-86-7**
PRO C **64545-12-6**, D **64578-20-7**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE Reaction was run neat. The 1, 4-adduct was the major product

RX(3) OF 43 2 A + 2 **G** ===> **H** + **I**



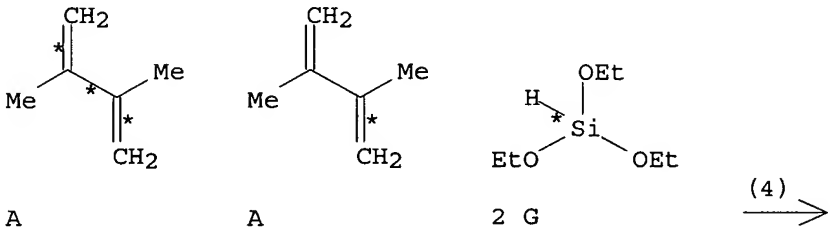
A A 2 G (3)



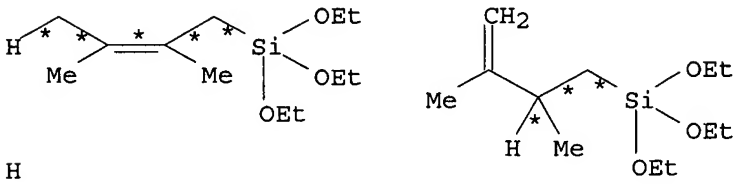
H I

RX(3) RCT A 513-81-5, G **998-30-1**
PRO H **63424-04-4**, I **64545-11-5**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat. The 1, 4-adduct was the major product

RX(4) OF 43 2 A + 2 **G** ===> **H** + **I**



A A 2 G (4)

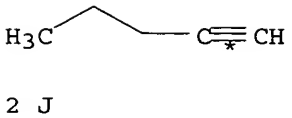


H I

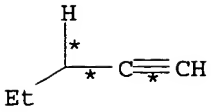
RX(4) RCT A 513-81-5, G **998-30-1**
PRO H **63424-04-4**, I **64545-11-5**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE Reaction was run neat. The 1, 4-adduct was the major product

RX(5) OF 43 3 J + 3 **B** ===> **K** + **L** +

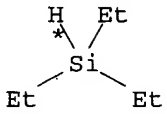
M



2 J

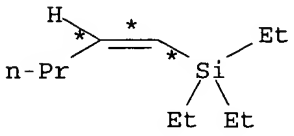


J

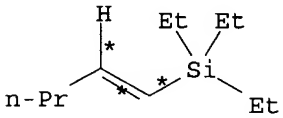


3 B

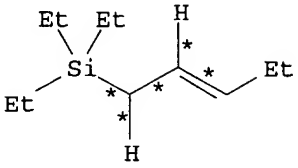
(5) ⟶



K



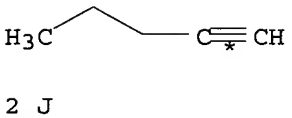
L



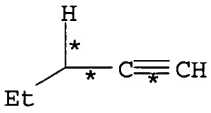
M

RX(5) RCT J 627-19-0, B **617-86-7**
PRO K **68928-08-5**, L **68928-07-4**, M **40962-02-5**
CAT **12246-51-4** Cyclooctene Ir

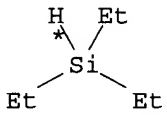
RX(6) OF 43 3 J + 3 **B** ===> **K** + **L** +
M



2 J

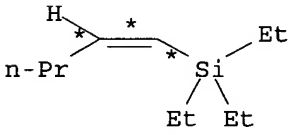


J

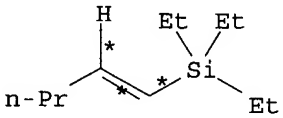


3 B

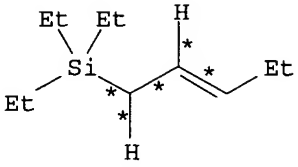
(6) ⟶



K



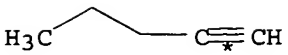
L



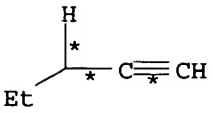
M

RX(6) RCT J 627-19-0, B **617-86-7**
PRO K **68928-08-5**, L **68928-07-4**, M **40962-02-5**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3

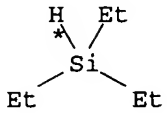
RX(7) OF 43 3 J + 3 **B** ===> **K** + **L** +
M



2 J

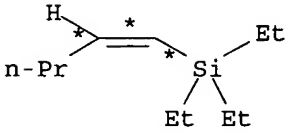


J

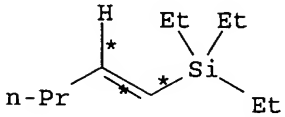


3 B

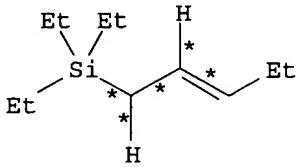
(7)



K



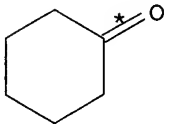
L



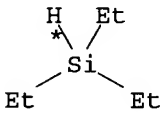
M

RX(7) RCT J 627-19-0, B **617-86-7**
PRO K **68928-08-5**, L **68928-07-4**, M **40962-02-5**
CAT **12246-51-4** Cyclooctene Ir, 6163-58-2 Tri-o-tolylphosphine

RX(10) OF 43 ...P + **B** ===> **T**

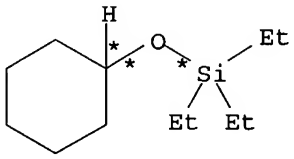


P



B

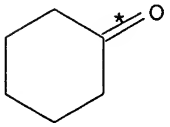
(10)



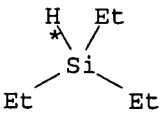
T

RX(10) RCT P 108-94-1, B **617-86-7**
PRO T **4419-18-5**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat

RX(11) OF 43 P + **B** ===> **T**

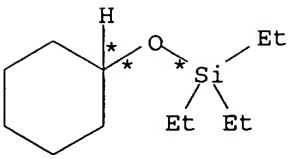


P



B

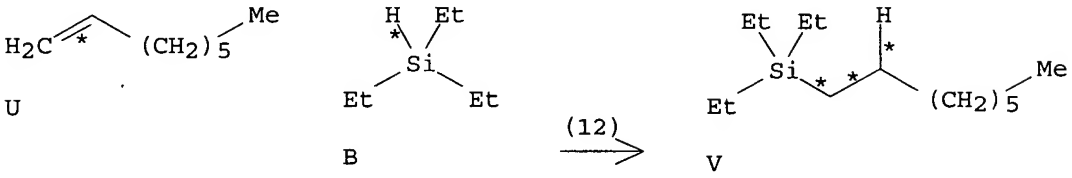
(11)



T

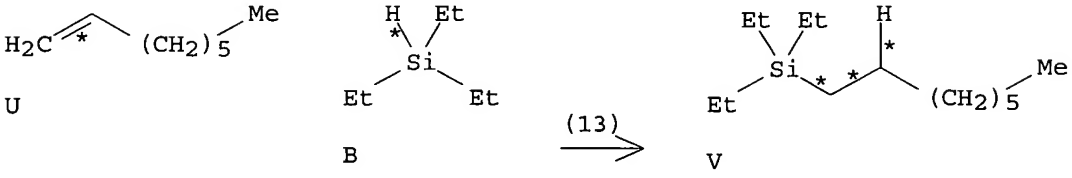
RX(11) RCT P 108-94-1, B **617-86-7**
PRO T **4419-18-5**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE Reaction was run neat

RX(12) OF 43 U + **B** ===> **V**



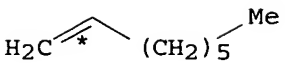
RX(12) RCT U 111-66-0, B **617-86-7**
PRO V **10175-53-8**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE Rxn was run neat

RX(13) OF 43 U + **B** ===> **V**

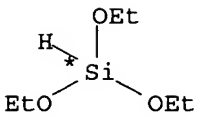


RX(13) RCT U 111-66-0, B **617-86-7**
PRO V **10175-53-8**
CAT **12246-51-4** Cyclooctene Ir, 6163-58-2
Tri-o-tolylphosphine
NTE Rxn was run neat

RX(14) OF 43 U + **G** ===> **W**

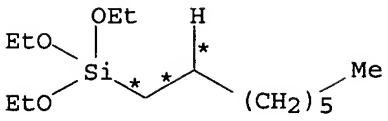


U



G

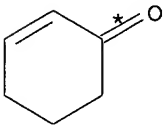
(14)



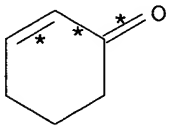
W

RX(14) RCT U 111-66-0, G **998-30-1**
PRO W **2943-75-1**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE Rxn was run neat

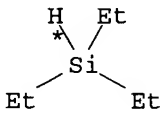
RX(17) OF 43 2 Z + 2 **B** ===> **AA** + **O**...



Z

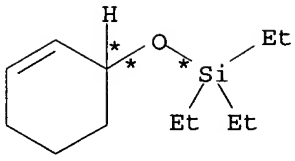


Z

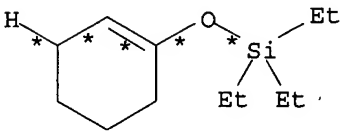


2 B

(17)



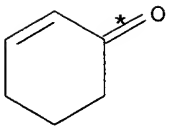
AA



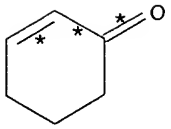
O

RX(17) RCT Z 930-68-7, B **617-86-7**
PRO AA **96474-45-2**, O **4342-22-7**
CAT **12246-51-4** Cyclooctene Ir
NTE The rxn was run neat. The 1,2-adduct was the major product

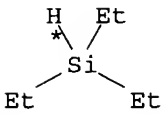
RX(18) OF 43 2 Z + 2 **B** ===> **AA** + **O**



Z

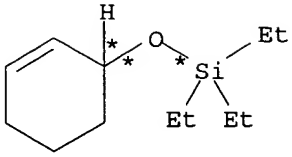


Z

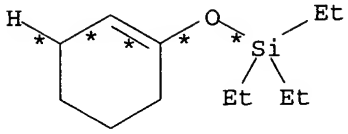


2 B

(18)



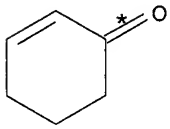
AA



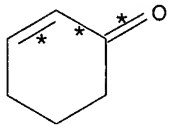
O

RX(18) RCT Z 930-68-7, B **617-86-7**
PRO AA **96474-45-2**, O **4342-22-7**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
NTE The rxn was run neat. The 1,2-adduct was the major product

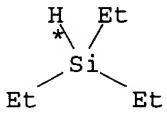
RX(19) OF 43 2 Z + 2 **B** ===> **AA** + **O**



Z

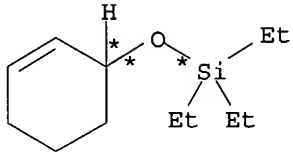


Z

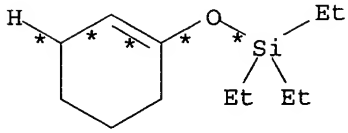


2 B

(19)



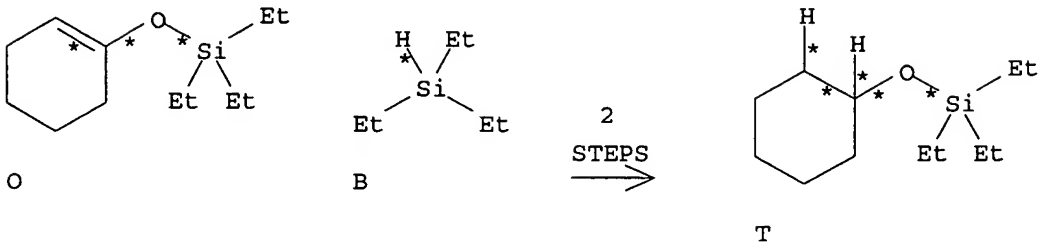
AA



O

RX(19) RCT Z 930-68-7, B **617-86-7**
PRO AA **96474-45-2**, O **4342-22-7**
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE The rxn was run neat. The 1,4-adduct was the major product

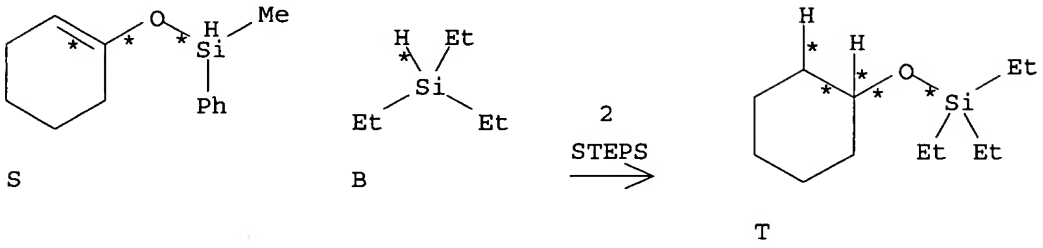
RX(31) OF 43 COMPOSED OF RX(8), RX(10)
RX(31) O + **B** ===> **T**



RX(8) RCT O 4342-22-7
RGT Q 584-08-7 K2CO3
PRO P 108-94-1
SOL 67-56-1 MeOH

RX(10) RCT P 108-94-1, B **617-86-7**
PRO T **4419-18-5**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat

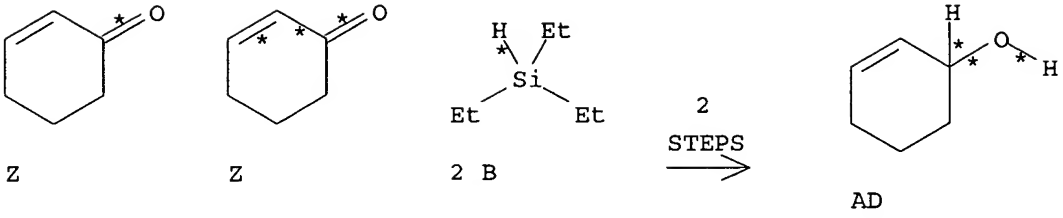
RX(33) OF 43 COMPOSED OF RX(9), RX(10)
RX(33) S + **B** ===> **T**



RX(9) RCT S 70790-00-0
RGT Q 584-08-7 K2CO3
PRO P 108-94-1
SOL 67-56-1 MeOH

RX(10) RCT P 108-94-1, B **617-86-7**
PRO T **4419-18-5**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat

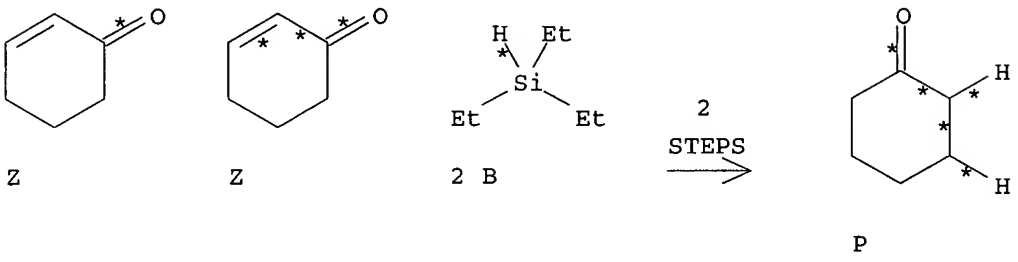
RX(35) OF 43 COMPOSED OF RX(17), RX(21)
RX(35) 2 Z + 2 **B** ===> **AD**



RX(17) RCT Z 930-68-7, B **617-86-7**
PRO AA 96474-45-2, O 4342-22-7
CAT **12246-51-4** Cyclooctene Ir
NTE The rxn was run neat. The 1,2-adduct was the major product

RX(21) RCT AA 96474-45-2
RGT Q 584-08-7 K2CO3
PRO AD **822-67-3**
SOL 67-56-1 MeOH

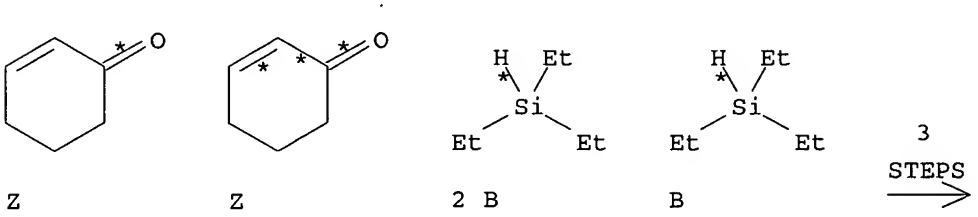
RX(36) OF 43 COMPOSED OF RX(17), RX(8)
RX(36) 2 Z + 2 **B** ===> **P**

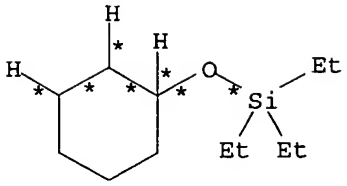


RX(17) RCT Z 930-68-7, B **617-86-7**
PRO AA 96474-45-2, O 4342-22-7
CAT **12246-51-4** Cyclooctene Ir
NTE The rxn was run neat. The 1,2-adduct was the major product

RX(8) RCT O 4342-22-7
RGT Q 584-08-7 K2CO3
PRO P **108-94-1**
SOL 67-56-1 MeOH

RX(40) OF 43 COMPOSED OF RX(17), RX(8), RX(10)
RX(40) 2 Z + 3 **B** ===> **T**





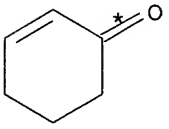
T

RX(17) RCT Z 930-68-7, B **617-86-7**
PRO AA 96474-45-2, O 4342-22-7
CAT **12246-51-4** Cyclooctene Ir
NTE The rxn was run neat. The 1,2-adduct was the major product

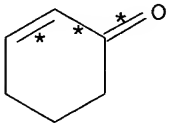
RX(8) RCT O 4342-22-7
RGT Q 584-08-7 K2CO3
PRO P 108-94-1
SOL 67-56-1 MeOH

RX(10) RCT P 108-94-1, B **617-86-7**
PRO T **4419-18-5**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat

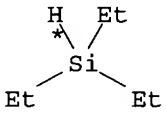
RX(41) OF 43 COMPOSED OF RX(17), RX(8), RX(28)
RX(41) 2 Z + 4 **B** + 2 F + E ===> **T** + **AS**



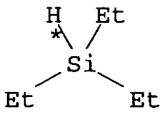
Z



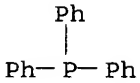
Z



2 B



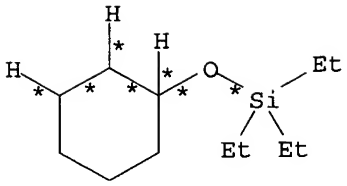
2 B



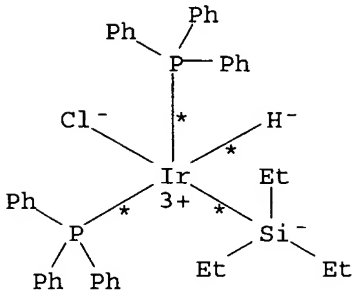
2 F

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

3
STEPS



T



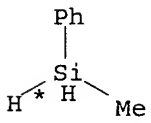
AS

RX(17) RCT Z 930-68-7, B **617-86-7**
PRO AA 96474-45-2, O 4342-22-7
CAT **12246-51-4** Cyclooctene Ir
NTE The rxn was run neat. The 1,2-adduct was the major product

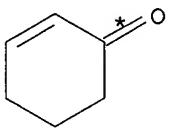
RX(8) RCT O 4342-22-7
RGT Q 584-08-7 K2CO3
PRO P 108-94-1
SOL 67-56-1 MeOH

RX(28) RCT P 108-94-1, B **617-86-7**, F 603-35-0, E 12246-51-4
PRO T **4419-18-5**, AS **75661-49-3**
NTE Only 2% of the hydrosilation product forms

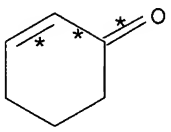
RX(42) OF 43 COMPOSED OF RX(22), RX(9), RX(10)
RX(42) 2 AE + 2 Z + **B** ===> **T**



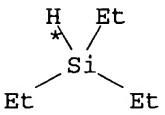
2 AE



Z

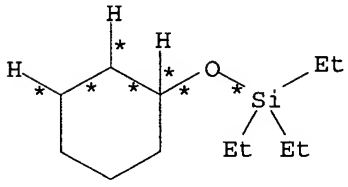


Z



B

3
STEPS



T

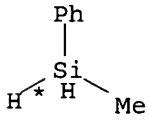
RX(22) RCT AE 766-08-5, Z 930-68-7
PRO AC 96474-46-3, S 70790-00-0
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3

NTE The rxn was run neat. The 1,2-adduct was the major product

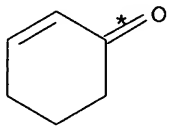
RX(9) RCT S 70790-00-0
RGT Q 584-08-7 K2CO3
PRO P 108-94-1
SOL 67-56-1 MeOH

RX(10) RCT P 108-94-1, B **617-86-7**
PRO T **4419-18-5**
CAT **12246-51-4** Cyclooctene Ir
NTE Reaction was run neat

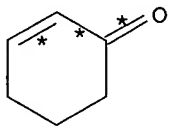
RX(43) OF 43 COMPOSED OF RX(22), RX(9), RX(28)
RX(43) 2 AE + 2 Z + 2 **B** + 2 F + E ===> **T** + **AS**



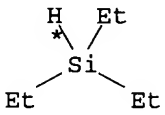
2 AE



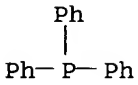
Z



Z



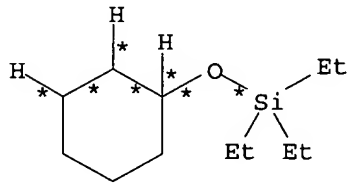
2 B



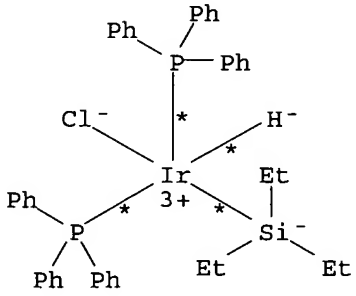
2 F

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

3 STEPS



T



AS

RX(22) RCT AE 766-08-5, Z 930-68-7
PRO AC 96474-46-3, S 70790-00-0
CAT **12246-51-4** Cyclooctene Ir, 603-35-0 PPh3
NTE The rxn was run neat. The 1,2-adduct was the major product

RX(9) RCT S 70790-00-0
RGT Q 584-08-7 K2CO3
PRO P 108-94-1
SOL 67-56-1 MeOH

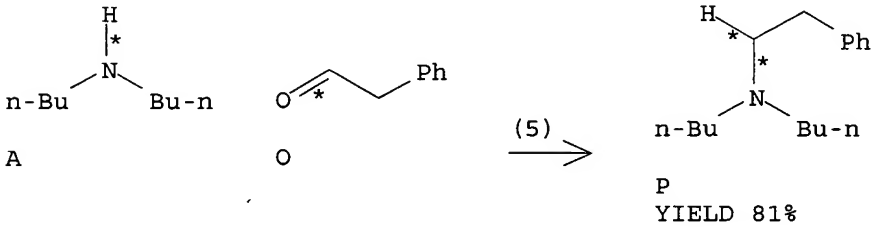
RX(28) RCT P 108-94-1, B **617-86-7**, F 603-35-0, E 12246-51-4
PRO T **4419-18-5**, AS **75661-49-3**
NTE Only 2% of the hydrosilation product forms

L64 ANSWER 15 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:373443 CASREACT
TITLE: Catalytic reductive alkylation of secondary amine with aldehyde and silane by an iridium compound
AUTHOR(S): Mizuta, Tomoya; Sakaguchi, Satoshi; Ishii, Yasutaka
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering High Technology Research Center, Kansai University, Suita, Osaka, 564-8680, Japan
SOURCE: Journal of Organic Chemistry (2005), 70(6), 2195-2199
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An efficient methodol. for the reductive alkylation of secondary amine with aldehyde and Et3SiH using an iridium complex as a catalyst has been developed. Treatment of dibutylamine with butyraldehyde and Et3SiH under the influence of a catalytic amount of [IrCl(cod)]2 gave tributylamine in quant. yield. In this reaction, no reduction of aldehyde took place. It was found that IrCl3, which was a starting material for preparation of iridium complexes such as [IrCl(cod)]2, acted as an efficient catalyst for the present reductive alkylation of amine. In addition, a cheaper, easy-to-handle, and environmentally friendly reducing reagent such as polymethylhydrosiloxane (PMHS) in place of Et3SiH was also useful. Thus, a variety of secondary amines could be alkylated by allowing them to react with aldehydes and PMHS in the presence of an iridium catalyst to afford the corresponding tertiary amines in good to excellent yields. From the deuterium label expts., it was revealed that silane and water, generated during the formation of enamine by the reaction of amine and aldehyde, behave as a hydrogen source. The catalytic cycle is also discussed.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(5) OF 12 A + O ===> **P**



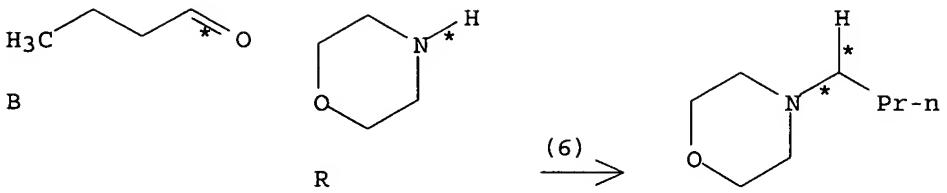
RX(5) RCT A 111-92-2, O 122-78-1

STAGE(1)
RGT Q **617-86-7** Et3SiH
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 123-91-1 Dioxane
CON 5 hours, 50 deg C

STAGE(2)
RGT E 7732-18-5 Water, F 60-29-7 Et2O

PRO P **5779-51-1**

RX(6) OF 12 B + R ===> **S**



YIELD 90%

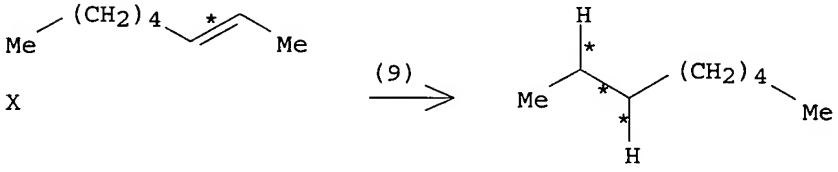
RX(6) RCT B 123-72-8, R 110-91-8

STAGE(1)
RGT Q **617-86-7** Et3SiH
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 123-91-1 Dioxane
CON 8 hours, 75 deg C

STAGE(2)
RGT E 7732-18-5 Water, F 60-29-7 Et2O

PRO S **1005-67-0**

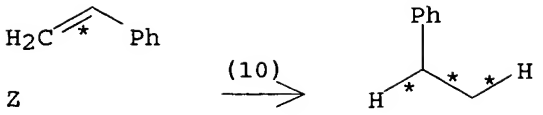
RX(9) OF 12 X ===> **Y**



YIELD 99%

RX(9) RCT X 111-67-1
RGT Q **617-86-7** Et3SiH, E 7732-18-5 Water
PRO Y **111-65-9**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 123-91-1 Dioxane
CON 8 hours, 75 deg C

RX(10) OF 12 Z ===> **AA**



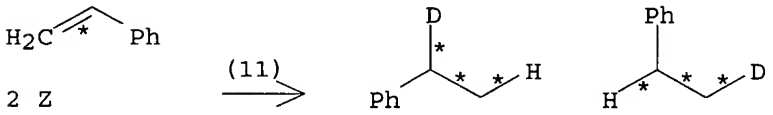
Z

(10)

AA
YIELD 99%

RX(10) RCT Z 100-42-5
RGT Q **617-86-7** Et3SiH, E 7732-18-5 Water
PRO AA **100-41-4**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 123-91-1 Dioxane
CON 8 hours, 75 deg C

RX(11) OF 12 2 Z ===> **AB** + **AC**



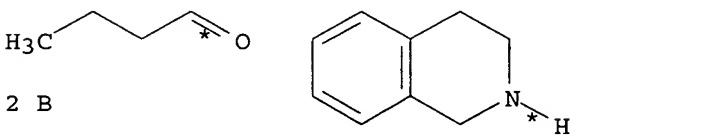
2 Z

(11)

AB AC

RX(11) RCT Z 100-42-5
RGT Q **617-86-7** Et3SiH, AD 7789-20-0 D2O
PRO AB **1861-02-5**, AC **1861-04-7**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 123-91-1 Dioxane
CON 8 hours, 75 deg C

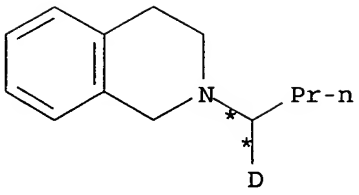
RX(12) OF 12 2 B + 2 V ===> **AE** + **AF**



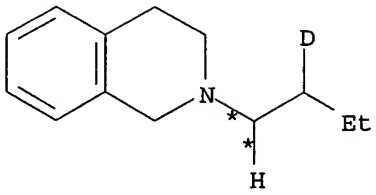
2 B

2 V

(12)



AE



AF

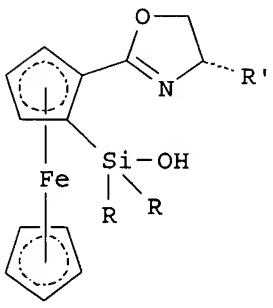
RX(12) RCT B 123-72-8, V 91-21-4

STAGE(1)
RGT AG **1631-33-0** Silane-d, triethyl-
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 123-91-1 Dioxane
CON 5 hours, 50 deg C

STAGE(2)
RGT E 7732-18-5 Water, F 60-29-7 Et2O

PRO AE **849592-25-2**, AF **849592-26-3**

L64 ANSWER 16 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 142:447278 CASREACT
TITLE: Organosilanols as Catalysts in Asymmetric Aryl Transfer Reactions
AUTHOR(S): Oezcubukcu, Salih; Schmidt, Frank; Bolm, Carsten
CORPORATE SOURCE: Institut fuer Organische Chemie, RWTH Aachen, Aachen, D-52074, Germany
SOURCE: Organic Letters (2005), 7(7), 1407-1409
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

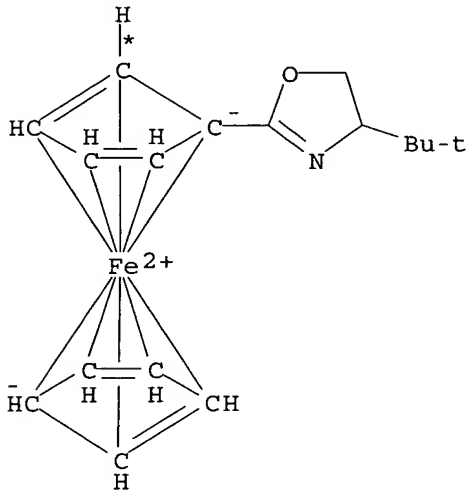


I

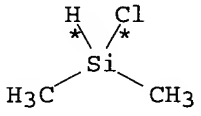
AB Various ferrocene-based organosilanols (I, R = CH3, i-Pr, Ph; R' = t-Bu, Ph, i-Pr, CH2Ph) have been synthesized in four steps starting from achiral ferrocene carboxylic acid. Applying these novel planar-chiral ferrocenes as catalysts in asym. Ph transfer reactions to substituted benzaldehydes afforded products with high enantiomeric excesses. The best result (91% ee) was achieved in the addition to p-chlorobenzaldehyde with organosilanol I (R = i-Pr, R' = t-Bu), which has a tert-Bu substituent on the oxazoline ring and an iso-Pr group on the silanol fragment.

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(23) OF 29 COMPOSED OF RX(1), RX(8)
RX(23) A + **B** ===> **R**



A



B

2 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 162157-02-0

STAGE(1)
RGT D 598-30-1 s-BuLi
SOL 109-99-9 THF, 110-82-7 Cyclohexane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C
SUBSTAGE(3) 2 hours, -78 deg C

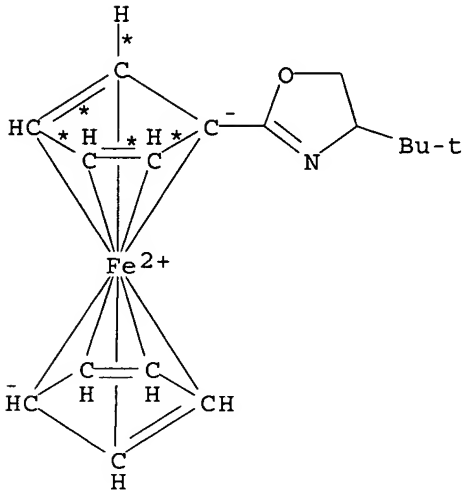
STAGE(2)
RCT B **1066-35-9**
CON overnight, -78 deg C -> room temperature

PRO C 851192-07-9
NTE stereoselective

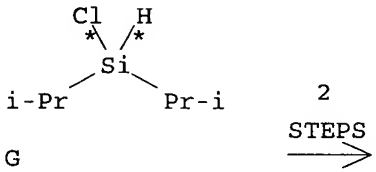
RX(8) RCT C 851192-07-9

RGT S 7732-18-5 Water, T 7782-44-7 O2
PRO R **851192-16-0**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON room temperature
NTE stereoselective

RX(24) OF 29 COMPOSED OF RX(2), RX(9)
RX(24) A + **G** ===> **W**

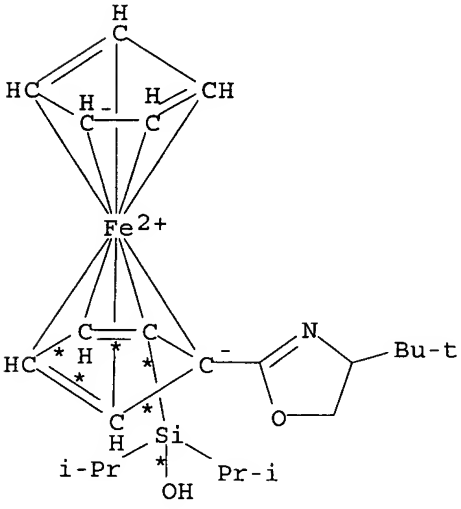


A



G

2 STEPS



W
YIELD 77%

RX(2) RCT A 162157-02-0

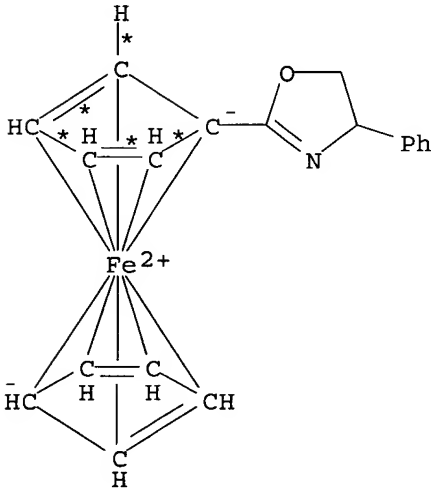
STAGE(1)
RGT D 598-30-1 s-BuLi
SOL 109-99-9 THF, 110-82-7 Cyclohexane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C
SUBSTAGE(3) 2 hours, -78 deg C

STAGE(2)
RCT G **2227-29-4**
CON overnight, -78 deg C -> room temperature

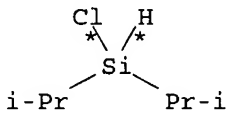
PRO H 851192-08-0
NTE stereoselective

RX(9) RCT H 851192-08-0
RGT S 7732-18-5 Water, T 7782-44-7 O2
PRO W **851192-18-2**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 60 deg C
NTE stereoselective

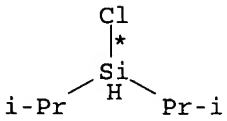
RX(26) OF 29 COMPOSED OF RX(4), RX(11)
RX(26) 2 K + 2 **G** ===> **Y**



2 K

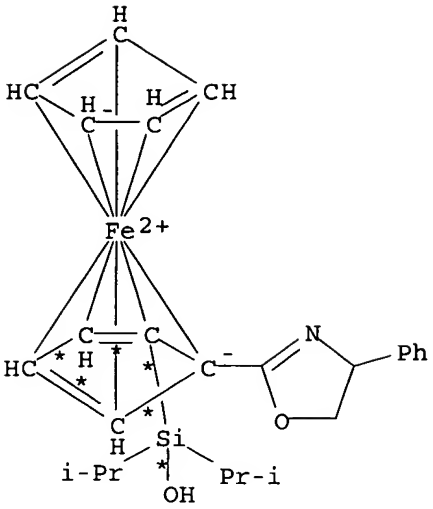


G



G

2
STEPS



Y
YIELD 57%

RX(4) RCT K 162157-04-2

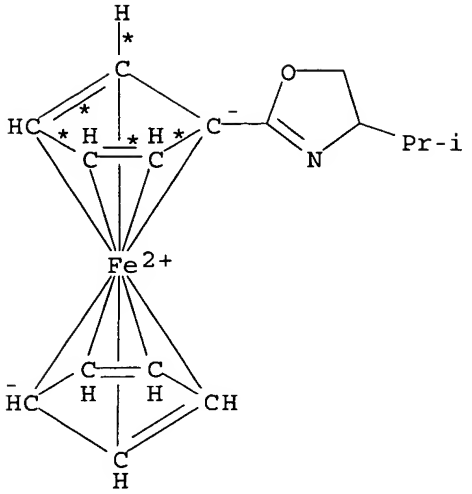
STAGE(1)
RGT D 598-30-1 s-BuLi
SOL 109-99-9 THF, 110-82-7 Cyclohexane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C
SUBSTAGE(3) 2 hours, -78 deg C

STAGE(2)
RCT G **2227-29-4**
CON overnight, -78 deg C -> room temperature

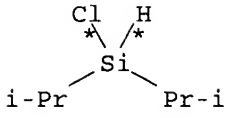
PRO L 851192-10-4, M 851192-34-2
NTE 70% overall yield, stereoselective

RX(11) RCT L 851192-10-4
RGT S 7732-18-5 Water, T 7782-44-7 O2
PRO Y **851192-23-9**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 60 deg C
NTE stereoselective

RX(28) OF 29 COMPOSED OF RX(6), RX(13)
RX(28) O + **G** ===> **AA**

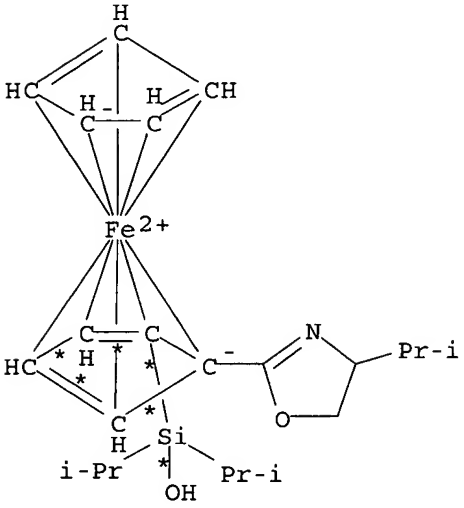


O



G

2 STEPS



AA
YIELD 65%

RX(6) RCT O 162157-03-1

STAGE(1)
RGT D 598-30-1 s-BuLi
SOL 109-99-9 THF, 110-82-7 Cyclohexane
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C
SUBSTAGE(3) 2 hours, -78 deg C

STAGE(2)
RCT G **2227-29-4**

CON overnight, -78 deg C -> room temperature

PRO P 851192-12-6
NTE stereoselective

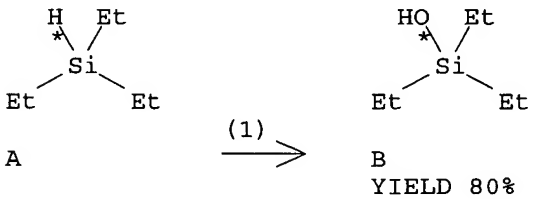
RX(13) RCT P 851192-12-6
RGT S 7732-18-5 Water, T 7782-44-7 O2
PRO AA **851192-26-2**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON room temperature
NTE stereoselective

L64 ANSWER 17 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:287436 CASREACT
TITLE: Highly Efficient Iridium-Catalyzed Oxidation of Organosilanes to Silanols
AUTHOR(S): Lee, Youngjun; Seomoon, Dong; Kim, Sundae; Han, Hoon; Chang, Sukbok; Lee, Phil Ho
CORPORATE SOURCE: Department of Chemistry, Kangwon National University, Chunchon, 200-701, S. Korea
SOURCE: Journal of Organic Chemistry (2004), 69(5), 1741-1743
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hydrolytic oxidation of organosilanes to the corresponding silanols can be performed highly efficiently with a catalyst system of [IrCl(C8H12)]2 under essentially neutral and mild conditions, and various types of silanols are produced in good to excellent yields. Oxidation of silanes R1R2R3SiH by exposure to air in the presence of 1 mol% of [IrCl(cod)]2 (cod = 1,2,5,6-η-1,5-cyclooctadiene) gave silanols R1R2R3SiOH (R1R2R3 = Et3, iBu3, Ph3, PhMe2, Ph2Me, Ph2H; R1 = R2 = Me, R3 = C18H37, 4-MeOC6H4, 4-BuC6H4, 4-MeC6H4CH2, PhCH:CH, Cl(CH2)3C.tplbond.C, 2-thienyl, 3-quinolinyl; R1 = R2 = iPr, R3 = PhC.tplbond.C; R1 = R2 = Ph, R3 = 2-thienyl) with yields generally higher than 80%. Oxidation of (+)-methyl(1-naphthyl)phenylsilane gave corresponding silanol with almost complete racemization.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 18 **A** ===> **B**



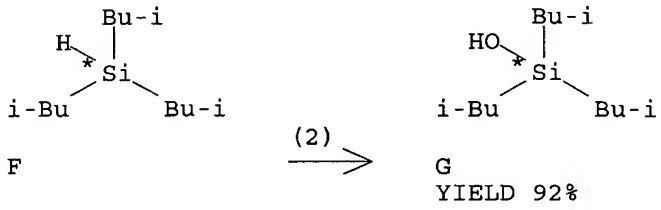
A

B
YIELD 80%

RX(1) RCT A **617-86-7**
RGT C 7732-18-5 Water
PRO B **597-52-4**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-

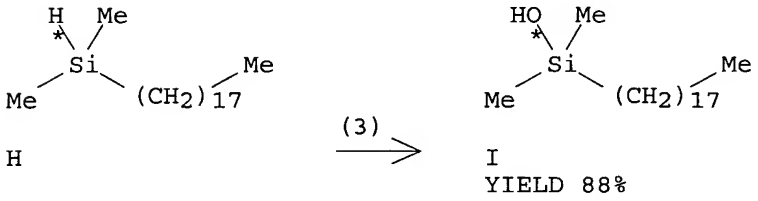
1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 4 hours, room temperature
NTE alternative reaction conditions gave lower yield

RX(2) OF 18 **F** ===> **G**



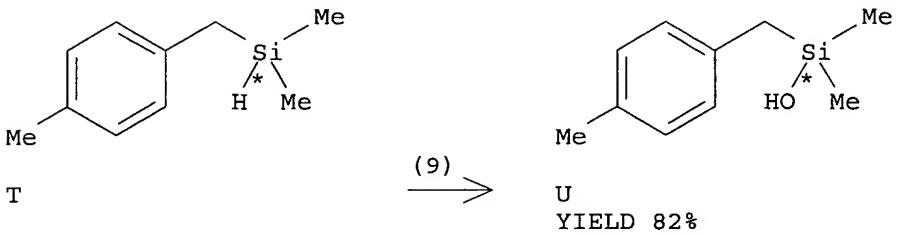
RX(2) RCT F **6485-81-0**
RGT C 7732-18-5 Water
PRO G **317374-14-4**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 2 hours, 80 deg C

RX(3) OF 18 **H** ===> **I**



RX(3) RCT H **32395-58-7**
RGT C 7732-18-5 Water
PRO I **58626-12-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 3 hours, room temperature

RX(9) OF 18 **T** ===> **U**



RX(9) RCT T **27856-33-3**
RGT C 7732-18-5 Water
PRO U **70430-64-7**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 0.5 hours, room temperature

RX(10) OF 18 **V** ===> **W**

V

W
YIELD 42%

RX(10) RCT V **119873-75-5**
RGT C 7732-18-5 Water
PRO W **119873-74-4**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 0.5 hours, room temperature

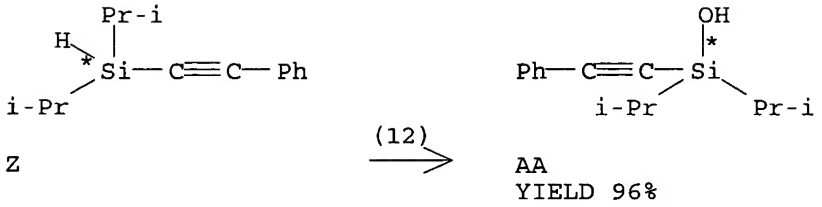
RX(11) OF 18 **X** ===> **Y**

X

Y
YIELD 22%

RX(11) RCT X **317374-20-2**
RGT C 7732-18-5 Water
PRO Y **317374-16-6**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 0.5 hours, room temperature

RX(12) OF 18 **Z** ===> **AA**



RX(12) RCT Z **317374-19-9**
RGT C 7732-18-5 Water
PRO AA **317374-15-5**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 75-05-8 MeCN
CON 12 hours, room temperature

L64 ANSWER 18 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:237929 CASREACT
TITLE: Enantioselective Total Synthesis of Borrelidin
AUTHOR(S): Duffey, Matthew O.; LeTiran, Arnaud; Morken, James P.
CORPORATE SOURCE: Department of Chemistry Venable and Kenan Laboratories, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290, USA
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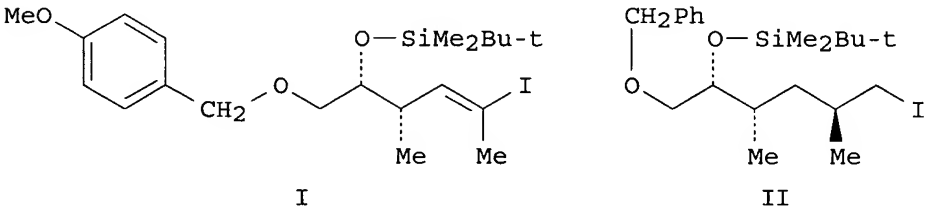
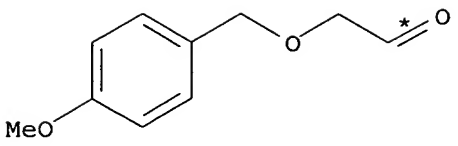
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

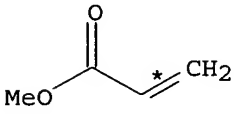


AB The first total synthesis of the natural product borrelidin is described. The propionate fragment of the mol. was concisely synthesized through catalytic enantioselective reductive aldol reactions, a catalytic Negishi coupling of vinyl iodide I with alkyl iodide II, and a catalytic directed hydrogenation. The propionate segment was then fused to the vinyl iodide fragment through a catalytic Sonogashira coupling. Subsequent catalytic hydrostannylation and catalytic cyanation allowed access to the target structure.
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(4) OF 594 U + V ===> **W**...

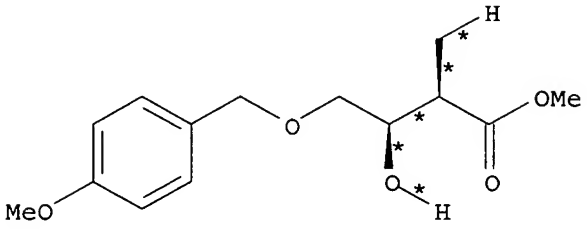


U



V

(4) →



W
YIELD 76%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

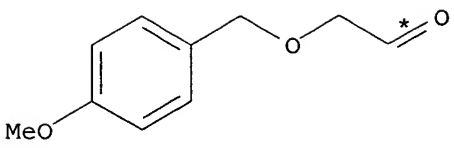
STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

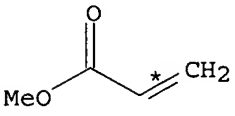
STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W **501419-01-8**
NTE stereoselective

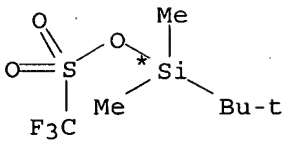
RX(50) OF 594 COMPOSED OF RX(4), RX(16)
RX(50) U + V + BY ===> **BZ**



U

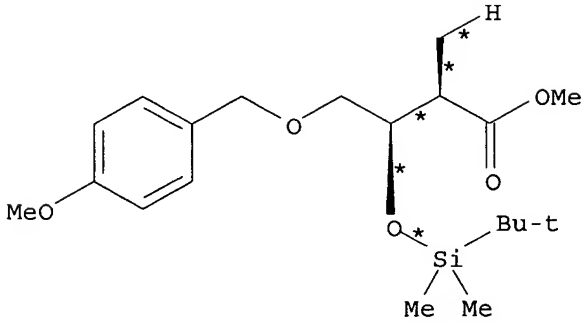


V



BY

2
STEPS
→



BZ
YIELD 90%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

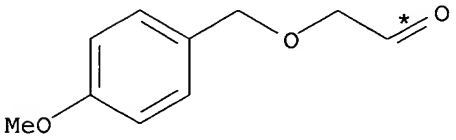
STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

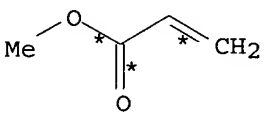
STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ **501419-19-8**

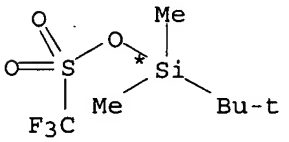
RX(98) OF 594 COMPOSED OF RX(4), RX(16), RX(17)
RX(98) U + V + BY ===> **CB**



U

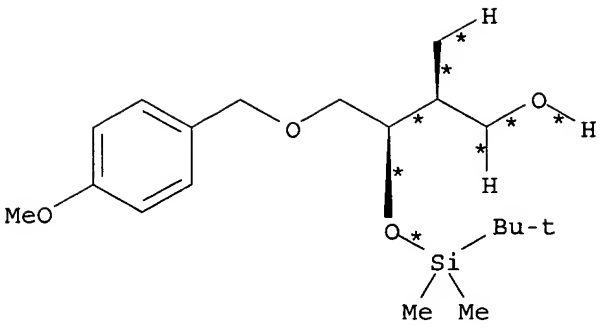


V



BY

3 STEPS



CB
YIELD 79%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

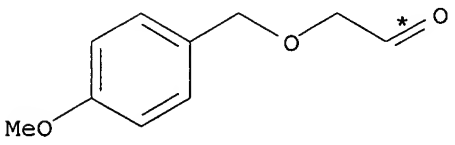
STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

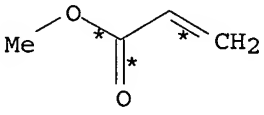
STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB **501419-20-1**

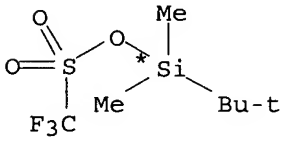
RX(119) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18)
RX(119) U + V + BY ===> **CD**



U

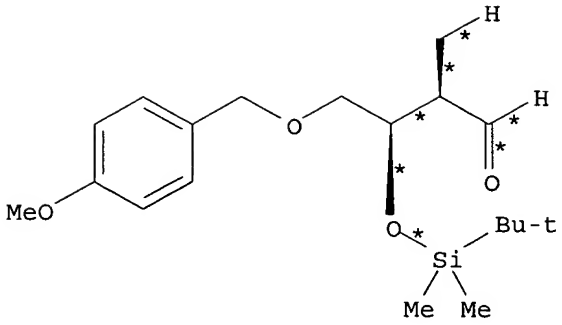


V



BY

4 STEPS



CD
YIELD 92%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

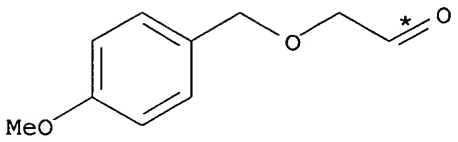
STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

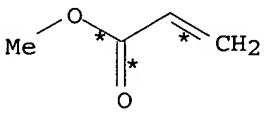
PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD **501419-21-2**
SOL 75-09-2 CH2Cl2
CON 90 minutes, room temperature

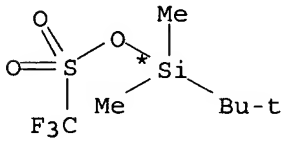
RX(195) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19)
RX(195) U + V + BY + CF ===> **CG**



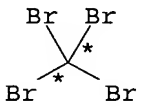
U



V

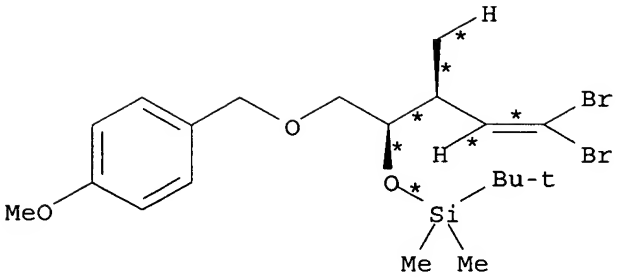


BY



CF

5 STEPS



CG
YIELD 94%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1
RGT CE 87413-09-0 Martin's reagent
PRO CD 501419-21-2
SOL 75-09-2 CH2Cl2
CON 90 minutes, room temperature

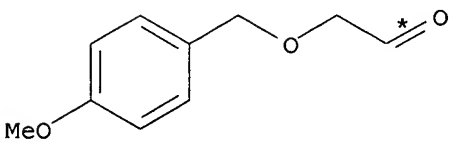
RX(19) RCT CF 558-13-4

STAGE(1)
RGT AI 603-35-0 PPh3
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> -78 deg C

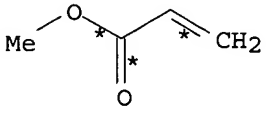
STAGE(2)
RCT CD 501419-21-2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 30 minutes, -78 deg C
SUBSTAGE(3) 10 minutes, 0 deg C

PRO CG **501419-22-3**

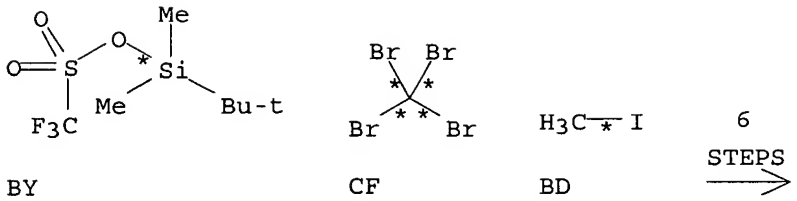
RX(270) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20)
RX(270) U + V + BY + CF + BD ===> **AB**



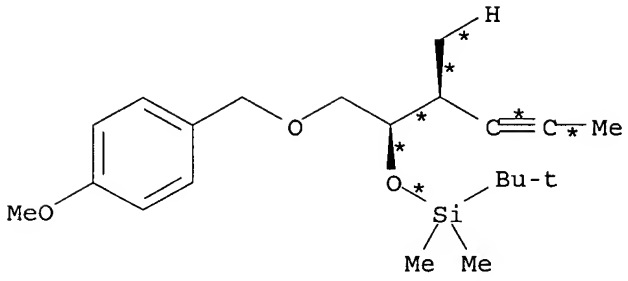
U



V



BY CF BD 6 STEPS



AB
YIELD 97%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

```
            STAGE(1)
               RGT  CA 108-48-5 2,6-Lutidine
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RCT  BY 69739-34-0
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 15 minutes, 0 deg C
                    SUBSTAGE(2) 0 deg C -> room temperature
                    SUBSTAGE(3) 1 hour, room temperature

            STAGE(3)
               RGT  G 144-55-8 NaHCO3
               SOL  7732-18-5 Water

         PRO  BZ 501419-19-8

RX(17)   RCT  BZ 501419-19-8

            STAGE(1)
               RGT  BF 1191-15-7 AlH(Bu-i)2
               SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 45 minutes, -78 deg C
                    SUBSTAGE(3) 30 minutes, 0 deg C

            STAGE(2)
               RGT  O 67-56-1 MeOH

            STAGE(3)
               RGT  CC 304-59-6 Rochelle salt
               SOL  7732-18-5 Water

         PRO  CB 501419-20-1

RX(18)   RCT  CB 501419-20-1
         RGT  CE 87413-09-0 Martin's reagent
         PRO  CD 501419-21-2
         SOL  75-09-2 CH2Cl2
         CON  90 minutes, room temperature

RX(19)   RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

         PRO  CG 501419-22-3
```

RX(20) RCT CG 501419-22-3

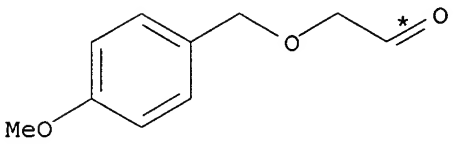
STAGE(1)
RGT CH 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) -78 deg C -> -25 deg C
SUBSTAGE(3) 1 hour, -25 deg C
SUBSTAGE(4) -25 deg C -> -78 deg C

STAGE(2)
RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

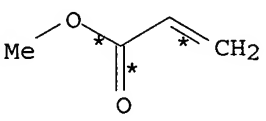
STAGE(3)
RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB **501419-23-4**

RX(273) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5)
RX(273) U + V + BY + CF + BD ===> **AC**



U



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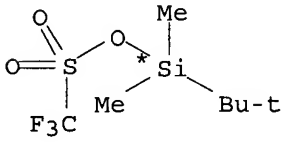
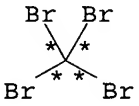
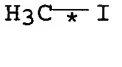


BY

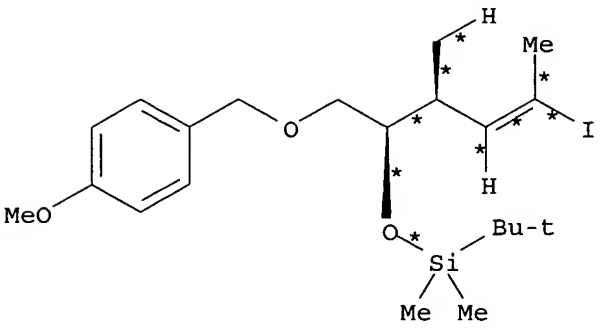


CF



BD

7 STEPS



AC
YIELD 89%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C

```
                SUBSTAGE(2) 0 deg C -> room temperature
                SUBSTAGE(3) 1 hour, room temperature

          STAGE(3)
             RGT  G 144-55-8 NaHCO3
             SOL  7732-18-5 Water

       PRO  BZ 501419-19-8

RX(17) RCT  BZ 501419-19-8

          STAGE(1)
             RGT  BF 1191-15-7 AlH(Bu-i)2
             SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
             CON  SUBSTAGE(1) -78 deg C
                  SUBSTAGE(2) 45 minutes, -78 deg C
                  SUBSTAGE(3) 30 minutes, 0 deg C

          STAGE(2)
             RGT  O 67-56-1 MeOH

          STAGE(3)
             RGT  CC 304-59-6 Rochelle salt
             SOL  7732-18-5 Water

       PRO  CB 501419-20-1

RX(18) RCT  CB 501419-20-1
       RGT  CE 87413-09-0 Martin's reagent
       PRO  CD 501419-21-2
       SOL  75-09-2 CH2Cl2
       CON  90 minutes, room temperature

RX(19) RCT  CF 558-13-4

          STAGE(1)
             RGT  AI 603-35-0 PPh3
             SOL  75-09-2 CH2Cl2
             CON  SUBSTAGE(1) 0 deg C
                  SUBSTAGE(2) 0 deg C -> -78 deg C

          STAGE(2)
             RCT  CD 501419-21-2
             SOL  75-09-2 CH2Cl2
             CON  SUBSTAGE(1) -78 deg C
                  SUBSTAGE(2) 30 minutes, -78 deg C
                  SUBSTAGE(3) 10 minutes, 0 deg C

       PRO  CG 501419-22-3

RX(20) RCT  CG 501419-22-3

          STAGE(1)
             RGT  CH 109-72-8 BuLi
             SOL  109-99-9 THF, 110-54-3 Hexane
             CON  SUBSTAGE(1) -78 deg C
                  SUBSTAGE(2) -78 deg C -> -25 deg C
                  SUBSTAGE(3) 1 hour, -25 deg C
                  SUBSTAGE(4) -25 deg C -> -78 deg C
```

STAGE(2)
RCT BD 74-88-4
SOL 109-99-9 THF
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)
RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

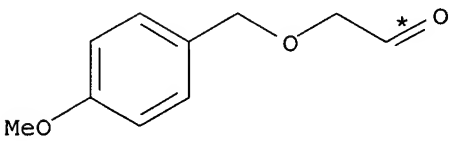
RX(5) RCT AB 501419-23-4

STAGE(1)
RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

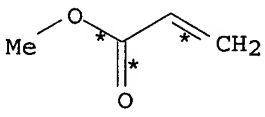
STAGE(2)
RGT AE 7553-56-2 I2
SOL 56-23-5 CCl4
CON 0 deg C

PRO AC **501419-02-9**
NTE in the dark, regioselective, stereoselective

RX(277) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9)
RX(277) U + V + BY + CF + BD + AT ===> **AU**



U



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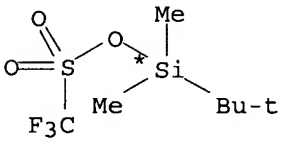
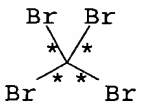


BY



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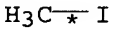

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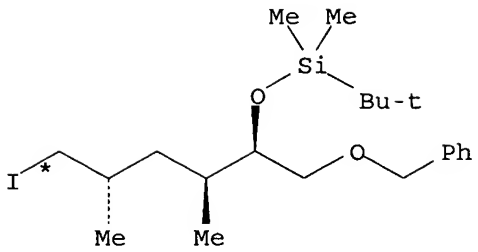
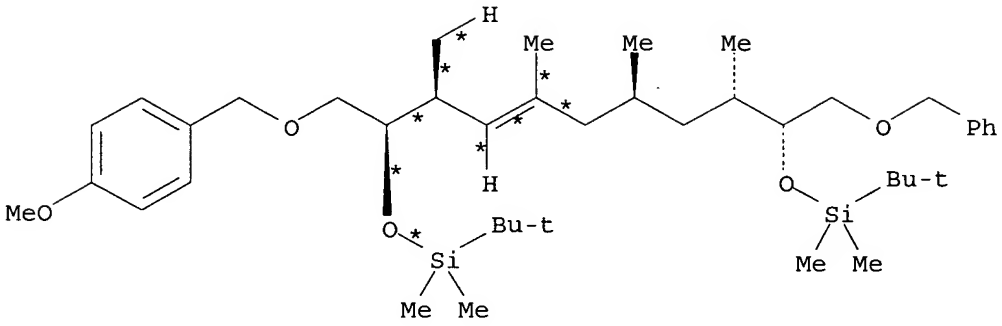


AT

8
STEPS



AU
YIELD 58%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

```
          PRO  W 501419-01-8
          NTE  stereoselective

RX(16)    RCT  W 501419-01-8

             STAGE(1)
                RGT  CA 108-48-5 2,6-Lutidine
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) room temperature
                     SUBSTAGE(2) room temperature -> 0 deg C

             STAGE(2)
                RCT  BY 69739-34-0
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 15 minutes, 0 deg C
                     SUBSTAGE(2) 0 deg C -> room temperature
                     SUBSTAGE(3) 1 hour, room temperature

             STAGE(3)
                RGT  G 144-55-8 NaHCO3
                SOL  7732-18-5 Water

          PRO  BZ 501419-19-8

RX(17)    RCT  BZ 501419-19-8

             STAGE(1)
                RGT  BF 1191-15-7 AlH(Bu-i)2
                SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 45 minutes, -78 deg C
                     SUBSTAGE(3) 30 minutes, 0 deg C

             STAGE(2)
                RGT  O 67-56-1 MeOH

             STAGE(3)
                RGT  CC 304-59-6 Rochelle salt
                SOL  7732-18-5 Water

          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

             STAGE(1)
                RGT  AI 603-35-0 PPh3
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 0 deg C
                     SUBSTAGE(2) 0 deg C -> -78 deg C

             STAGE(2)
                RCT  CD 501419-21-2
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) -78 deg C
```

```
                SUBSTAGE(2) 30 minutes, -78 deg C
                SUBSTAGE(3) 10 minutes, 0 deg C

          PRO   CG 501419-22-3

RX(20)    RCT   CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

            STAGE(3)
               RGT  AQ 12125-02-9 NH4Cl
               SOL  7732-18-5 Water

          PRO   AB 501419-23-4

RX(5)     RCT   AB 501419-23-4

            STAGE(1)
               RGT  AD 37342-97-5 Hydrozirconocene Cl
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 2 hours, room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RGT  AE 7553-56-2 I2
               SOL  56-23-5 CCl4
               CON  0 deg C

          PRO   AC 501419-02-9
          NTE   in the dark, regioselective, stereoselective

RX(9)     RCT   AT 501419-06-3

            STAGE(1)
               RGT  AV 7646-85-7 ZnCl2
               SOL  60-29-7 Et2O
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> -78 deg C

            STAGE(2)
               RGT  AW 594-19-4 t-BuLi
               SOL  110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 5 minutes, -78 deg C
                    SUBSTAGE(3) 1 hour, room temperature

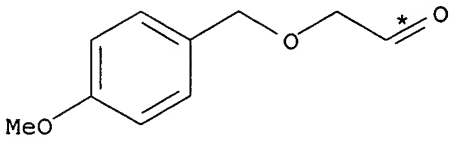
            STAGE(3)
               RCT  AC 501419-02-9
```

CAT 14221-01-3 Pd(PPh3)4
CON 16 hours, room temperature

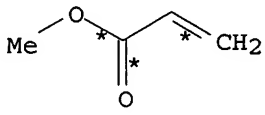
STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU **501419-08-5**
NTE modified Negishi coupling, stage three in the dark

RX(386) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24)
RX(386) U + V + BY + CF + BD + AT ===> **AY**



U



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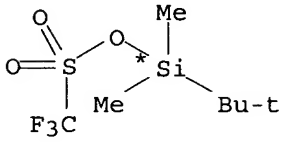
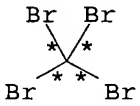


BY



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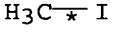
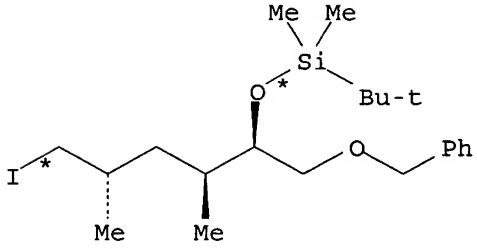
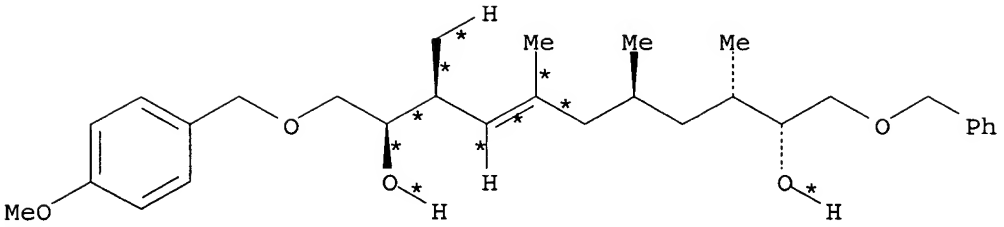


BD



AT

9
STEPS



AY
YIELD 87%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)

```
            RGT  G 144-55-8 NaHCO3
            SOL  7732-18-5 Water

         PRO  BZ 501419-19-8

RX(17)   RCT  BZ 501419-19-8

           STAGE(1)
              RGT  BF 1191-15-7 AlH(Bu-i)2
              SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
              CON  SUBSTAGE(1) -78 deg C
                   SUBSTAGE(2) 45 minutes, -78 deg C
                   SUBSTAGE(3) 30 minutes, 0 deg C

           STAGE(2)
              RGT  O 67-56-1 MeOH

           STAGE(3)
              RGT  CC 304-59-6 Rochelle salt
              SOL  7732-18-5 Water

         PRO  CB 501419-20-1

RX(18)   RCT  CB 501419-20-1
         RGT  CE 87413-09-0 Martin's reagent
         PRO  CD 501419-21-2
         SOL  75-09-2 CH2Cl2
         CON  90 minutes, room temperature

RX(19)   RCT  CF 558-13-4

           STAGE(1)
              RGT  AI 603-35-0 PPh3
              SOL  75-09-2 CH2Cl2
              CON  SUBSTAGE(1) 0 deg C
                   SUBSTAGE(2) 0 deg C -> -78 deg C

           STAGE(2)
              RCT  CD 501419-21-2
              SOL  75-09-2 CH2Cl2
              CON  SUBSTAGE(1) -78 deg C
                   SUBSTAGE(2) 30 minutes, -78 deg C
                   SUBSTAGE(3) 10 minutes, 0 deg C

         PRO  CG 501419-22-3

RX(20)   RCT  CG 501419-22-3

           STAGE(1)
              RGT  CH 109-72-8 BuLi
              SOL  109-99-9 THF, 110-54-3 Hexane
              CON  SUBSTAGE(1) -78 deg C
                   SUBSTAGE(2) -78 deg C -> -25 deg C
                   SUBSTAGE(3) 1 hour, -25 deg C
                   SUBSTAGE(4) -25 deg C -> -78 deg C

           STAGE(2)
              RCT  BD 74-88-4
              SOL  109-99-9 THF
              CON  SUBSTAGE(1) -78 deg C
```

SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

STAGE(3)
RGT AQ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO AB 501419-23-4

RX(5) RCT AB 501419-23-4

STAGE(1)
RGT AD 37342-97-5 Hydrozirconocene Cl
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 2 hours, room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RGT AE 7553-56-2 I2
SOL 56-23-5 CCl4
CON 0 deg C

PRO AC 501419-02-9
NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)
RGT AV 7646-85-7 ZnCl2
SOL 60-29-7 Et2O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)
RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh3)4
CON 16 hours, room temperature

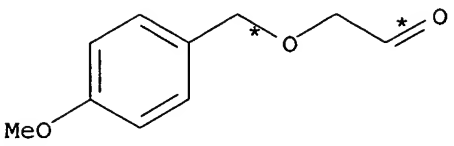
STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

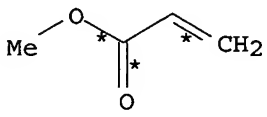
RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu4N.F
PRO AY **501419-27-8**
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(414) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20),

RX(5), RX(9), RX(24), RX(10), RX(25), RX(26)
RX(414) U + V + 3 BY + CF + BD + AT ===> CO



U



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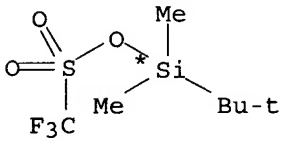
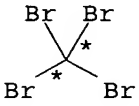


3 BY



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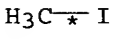
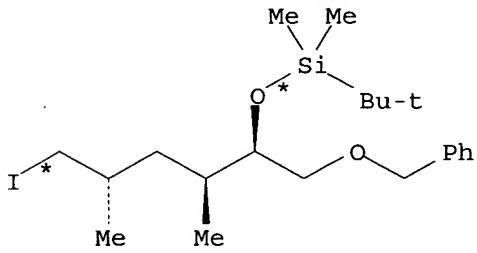
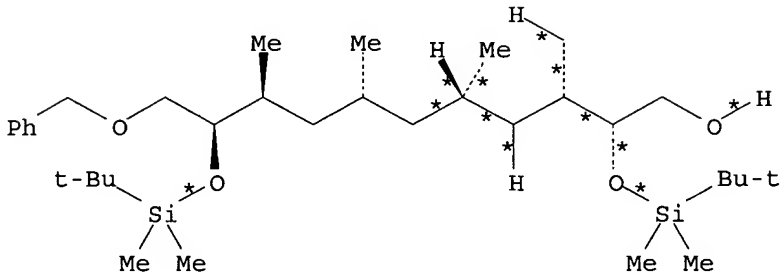


BD



AT

12
STEPS



CO
YIELD 93%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-

[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3**
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

```
          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

            STAGE(3)
               RGT  AQ 12125-02-9 NH4Cl
               SOL  7732-18-5 Water

          PRO  AB 501419-23-4

RX(5)     RCT  AB 501419-23-4

            STAGE(1)
               RGT  AD 37342-97-5 Hydrozirconocene Cl
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 2 hours, room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RGT  AE 7553-56-2 I2
               SOL  56-23-5 CCl4
               CON  0 deg C
```

```
          PRO  AC 501419-02-9
          NTE  in the dark, regioselective, stereoselective

RX(9)     RCT  AT 501419-06-3

            STAGE(1)
               RGT  AV 7646-85-7 ZnCl2
               SOL  60-29-7 Et2O
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> -78 deg C

            STAGE(2)
               RGT  AW 594-19-4 t-BuLi
               SOL  110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 5 minutes, -78 deg C
                    SUBSTAGE(3) 1 hour, room temperature

            STAGE(3)
               RCT  AC 501419-02-9
               CAT  14221-01-3 Pd(PPh3)4
               CON  16 hours, room temperature

            STAGE(4)
               RGT  K 7732-18-5 Water
               SOL  7732-18-5 Water

          PRO  AU 501419-08-5
          NTE  modified Negishi coupling, stage three in the dark

RX(24)    RCT  AU 501419-08-5
          RGT  CM 429-41-4 Bu4N.F
          PRO  AY 501419-27-8
          SOL  109-99-9 THF
          CON  20 hours, room temperature
          NTE  mol. sieves

RX(10)    RCT  AY 501419-27-8
          RGT  BA 1333-74-0 H2
          PRO  AZ 501419-10-9
          CAT  82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-
               diene][1,4-butanediylbis[diphenylphosphine-κP]]-,
               tetrafluoroborate(1-)
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) 4 hours, room temperature, 700 psi
          NTE  high pressure, stereoselective

RX(25)    RCT  AZ 501419-10-9, BY 69739-34-0

            STAGE(1)
               RGT  CA 108-48-5 2,6-Lutidine
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature -> 0 deg C
                    SUBSTAGE(2) 5 minutes, 0 deg C
                    SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

            STAGE(2)
               RGT  G 144-55-8 NaHCO3
```

SOL 7732-18-5 Water

PRO CN 501419-28-9

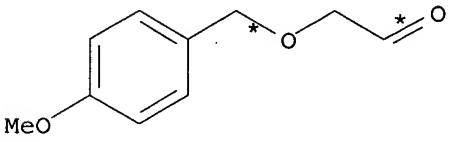
RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO **501419-29-0**
NTE chemoselective, buffered soln.

RX(415) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(27)
RX(415) U + V + 3 BY + CF + BD + AT + CQ ===> **CR**



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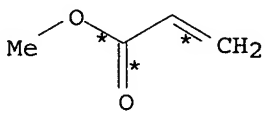

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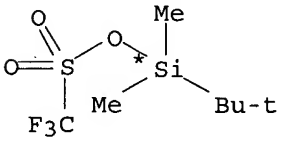
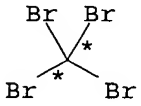


3 BY



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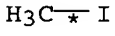

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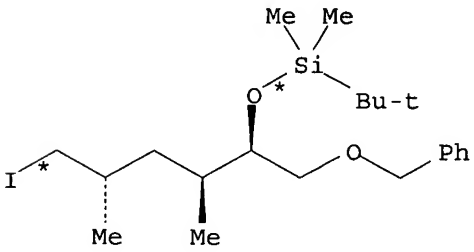

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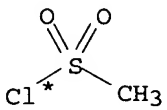
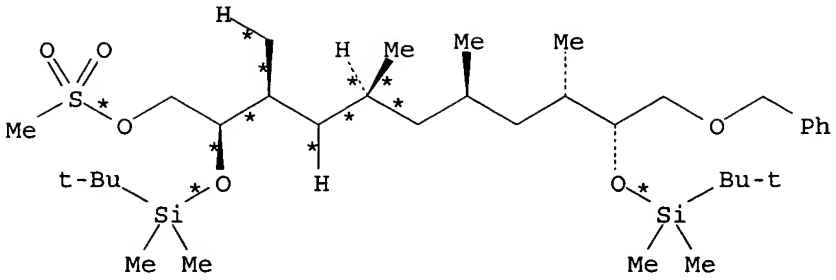


CQ

13 STEPS



CR

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

```
            STAGE(3)
               RGT  G 144-55-8 NaHCO3
               SOL  7732-18-5 Water

          PRO  BZ 501419-19-8

RX(17)    RCT  BZ 501419-19-8

            STAGE(1)
               RGT  BF 1191-15-7 AlH(Bu-i)2
               SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 45 minutes, -78 deg C
                    SUBSTAGE(3) 30 minutes, 0 deg C

            STAGE(2)
               RGT  O 67-56-1 MeOH

            STAGE(3)
               RGT  CC 304-59-6 Rochelle salt
               SOL  7732-18-5 Water

          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
```

```
            CON  SUBSTAGE(1) -78 deg C
                 SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

          STAGE(3)
            RGT  AQ 12125-02-9 NH4Cl
            SOL  7732-18-5 Water

        PRO  AB 501419-23-4

RX(5)   RCT  AB 501419-23-4

          STAGE(1)
            RGT  AD 37342-97-5 Hydrozirconocene Cl
            SOL  75-09-2 CH2Cl2
            CON  SUBSTAGE(1) 2 hours, room temperature
                 SUBSTAGE(2) room temperature -> 0 deg C

          STAGE(2)
            RGT  AE 7553-56-2 I2
            SOL  56-23-5 CCl4
            CON  0 deg C

        PRO  AC 501419-02-9
        NTE  in the dark, regioselective, stereoselective

RX(9)   RCT  AT 501419-06-3

          STAGE(1)
            RGT  AV 7646-85-7 ZnCl2
            SOL  60-29-7 Et2O
            CON  SUBSTAGE(1) room temperature
                 SUBSTAGE(2) room temperature -> -78 deg C

          STAGE(2)
            RGT  AW 594-19-4 t-BuLi
            SOL  110-54-3 Hexane
            CON  SUBSTAGE(1) -78 deg C
                 SUBSTAGE(2) 5 minutes, -78 deg C
                 SUBSTAGE(3) 1 hour, room temperature

          STAGE(3)
            RCT  AC 501419-02-9
            CAT  14221-01-3 Pd(PPh3)4
            CON  16 hours, room temperature

          STAGE(4)
            RGT  K 7732-18-5 Water
            SOL  7732-18-5 Water

        PRO  AU 501419-08-5
        NTE  modified Negishi coupling, stage three in the dark

RX(24)  RCT  AU 501419-08-5
        RGT  CM 429-41-4 Bu4N.F
        PRO  AY 501419-27-8
        SOL  109-99-9 THF
        CON  20 hours, room temperature
        NTE  mol. sieves

RX(10)  RCT  AY 501419-27-8
```

RGT BA 1333-74-0 H2
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

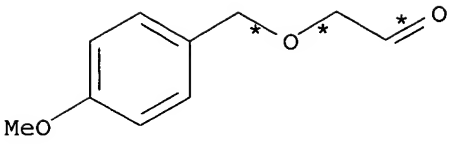
RX(27) RCT CO 501419-29-0, CQ 124-63-0

STAGE(1)
RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)
RGT K 7732-18-5 Water

PRO CR **501419-30-3**

RX(416) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29)
RX(416) U + V + 3 BY + CF + BD + AT ===> **CU**



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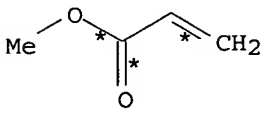
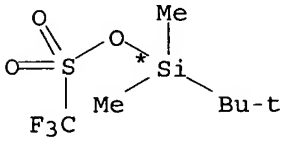
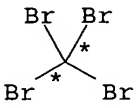


V



3 BY



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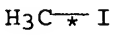

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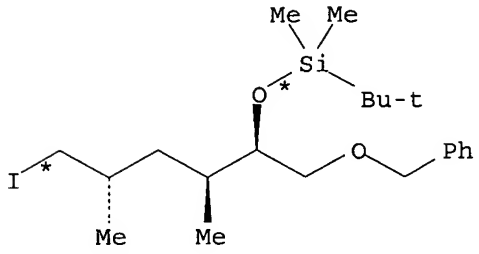
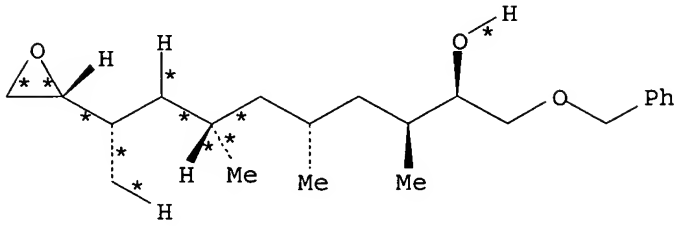


AT

13
STEPS



CU
YIELD 98%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl

CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

PRO CB 501419-20-1

RX(18) RCT CB 501419-20-1

```
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

            STAGE(3)
               RGT  AQ 12125-02-9 NH4Cl
               SOL  7732-18-5 Water

          PRO  AB 501419-23-4

RX(5)     RCT  AB 501419-23-4

            STAGE(1)
               RGT  AD 37342-97-5 Hydrozirconocene Cl
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 2 hours, room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RGT  AE 7553-56-2 I2
               SOL  56-23-5 CCl4
               CON  0 deg C

          PRO  AC 501419-02-9
          NTE  in the dark, regioselective, stereoselective
```

```
RX(9)     RCT  AT 501419-06-3

            STAGE(1)
               RGT  AV 7646-85-7 ZnCl2
               SOL  60-29-7 Et2O
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> -78 deg C

            STAGE(2)
               RGT  AW 594-19-4 t-BuLi
               SOL  110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 5 minutes, -78 deg C
                    SUBSTAGE(3) 1 hour, room temperature

            STAGE(3)
               RCT  AC 501419-02-9
               CAT  14221-01-3 Pd(PPh3)4
               CON  16 hours, room temperature

            STAGE(4)
               RGT  K 7732-18-5 Water
               SOL  7732-18-5 Water

          PRO  AU 501419-08-5
          NTE  modified Negishi coupling, stage three in the dark

RX(24)    RCT  AU 501419-08-5
          RGT  CM 429-41-4 Bu4N.F
          PRO  AY 501419-27-8
          SOL  109-99-9 THF
          CON  20 hours, room temperature
          NTE  mol. sieves

RX(10)    RCT  AY 501419-27-8
          RGT  BA 1333-74-0 H2
          PRO  AZ 501419-10-9
          CAT  82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-
               diene][1,4-butanediylbis[diphenylphosphine-κP]]-,
               tetrafluoroborate(1-)
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) 4 hours, room temperature, 700 psi
          NTE  high pressure, stereoselective

RX(25)    RCT  AZ 501419-10-9, BY 69739-34-0

            STAGE(1)
               RGT  CA 108-48-5 2,6-Lutidine
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature -> 0 deg C
                    SUBSTAGE(2) 5 minutes, 0 deg C
                    SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

            STAGE(2)
               RGT  G 144-55-8 NaHCO3
               SOL  7732-18-5 Water

          PRO  CN 501419-28-9
```

RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)
RGT CQ 124-63-0 MeSO2Cl, D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

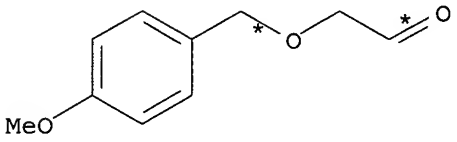
STAGE(2)
RGT K 7732-18-5 Water

STAGE(3)
RGT CT 7664-39-3 HF
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

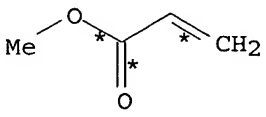
STAGE(4)
RGT BJ 584-08-7 K2CO3
SOL 67-56-1 MeOH
CON 45 minutes, room temperature

PRO CU **501419-32-5**

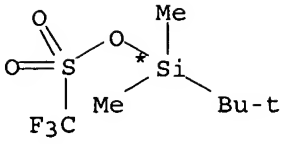
RX(417) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(27), RX(28)
RX(417) U + V + 3 BY + CF + BD + AT + CQ ===> **CS**



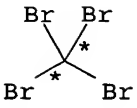
U



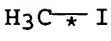
V



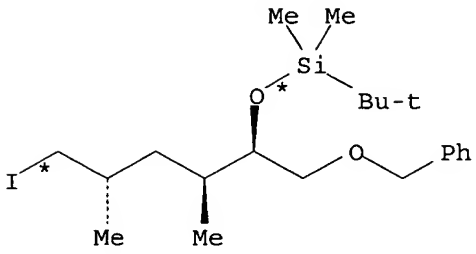
3 BY



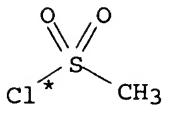
CF



BD

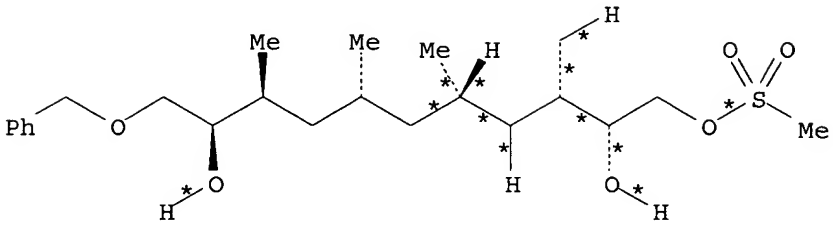


AT



CQ

14 STEPS



CS

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3**
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

```
            STAGE(4)
               RGT  N 7647-01-0 HCl
               SOL  109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
               CON  30 minutes, room temperature

            PRO  W 501419-01-8
            NTE  stereoselective

RX(16)      RCT  W 501419-01-8

            STAGE(1)
               RGT  CA 108-48-5 2,6-Lutidine
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RCT  BY 69739-34-0
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 15 minutes, 0 deg C
                    SUBSTAGE(2) 0 deg C -> room temperature
                    SUBSTAGE(3) 1 hour, room temperature

            STAGE(3)
               RGT  G 144-55-8 NaHCO3
               SOL  7732-18-5 Water

            PRO  BZ 501419-19-8

RX(17)      RCT  BZ 501419-19-8

            STAGE(1)
               RGT  BF 1191-15-7 AlH(Bu-i)2
               SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 45 minutes, -78 deg C
                    SUBSTAGE(3) 30 minutes, 0 deg C

            STAGE(2)
               RGT  O 67-56-1 MeOH

            STAGE(3)
               RGT  CC 304-59-6 Rochelle salt
               SOL  7732-18-5 Water

            PRO  CB 501419-20-1

RX(18)      RCT  CB 501419-20-1
            RGT  CE 87413-09-0 Martin's reagent
            PRO  CD 501419-21-2
            SOL  75-09-2 CH2Cl2
            CON  90 minutes, room temperature

RX(19)      RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C
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```
            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

         PRO   CG 501419-22-3

RX(20)   RCT   CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

            STAGE(3)
               RGT  AQ 12125-02-9 NH4Cl
               SOL  7732-18-5 Water

         PRO   AB 501419-23-4

RX(5)    RCT   AB 501419-23-4

            STAGE(1)
               RGT  AD 37342-97-5 Hydrozirconocene Cl
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 2 hours, room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RGT  AE 7553-56-2 I2
               SOL  56-23-5 CCl4
               CON  0 deg C

         PRO   AC 501419-02-9
         NTE   in the dark, regioselective, stereoselective

RX(9)    RCT   AT 501419-06-3

            STAGE(1)
               RGT  AV 7646-85-7 ZnCl2
               SOL  60-29-7 Et2O
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> -78 deg C

            STAGE(2)
               RGT  AW 594-19-4 t-BuLi
               SOL  110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
```

```
                SUBSTAGE(2) 5 minutes, -78 deg C
                SUBSTAGE(3) 1 hour, room temperature

          STAGE(3)
             RCT  AC 501419-02-9
             CAT  14221-01-3 Pd(PPh3)4
             CON  16 hours, room temperature

          STAGE(4)
             RGT  K 7732-18-5 Water
             SOL  7732-18-5 Water

        PRO  AU 501419-08-5
        NTE  modified Negishi coupling, stage three in the dark

RX(24)  RCT  AU 501419-08-5
        RGT  CM 429-41-4 Bu4N.F
        PRO  AY 501419-27-8
        SOL  109-99-9 THF
        CON  20 hours, room temperature
        NTE  mol. sieves

RX(10)  RCT  AY 501419-27-8
        RGT  BA 1333-74-0 H2
        PRO  AZ 501419-10-9
        CAT  82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-
             diene][1,4-butanediylbis[diphenylphosphine-κP]]-,
             tetrafluoroborate(1-)
        SOL  75-09-2 CH2Cl2
        CON  SUBSTAGE(1) room temperature
             SUBSTAGE(2) 4 hours, room temperature, 700 psi
        NTE  high pressure, stereoselective

RX(25)  RCT  AZ 501419-10-9, BY 69739-34-0

          STAGE(1)
             RGT  CA 108-48-5 2,6-Lutidine
             SOL  75-09-2 CH2Cl2
             CON  SUBSTAGE(1) room temperature -> 0 deg C
                  SUBSTAGE(2) 5 minutes, 0 deg C
                  SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

          STAGE(2)
             RGT  G 144-55-8 NaHCO3
             SOL  7732-18-5 Water

        PRO  CN 501419-28-9

RX(26)  RCT  CN 501419-28-9

          STAGE(1)
             RGT  CP 84-58-2 DDQ
             SOL  75-09-2 CH2Cl2, 7732-18-5 Water
             CON  1 hour, room temperature, pH 7

          STAGE(2)
             RGT  G 144-55-8 NaHCO3
             SOL  7732-18-5 Water

        PRO  CO 501419-29-0
```

NTE chemoselective, buffered soln.

RX(27) RCT CO 501419-29-0, CQ 124-63-0

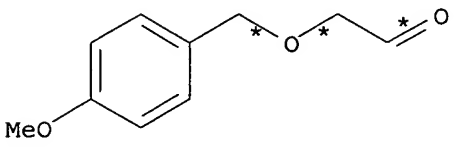
STAGE(1)
RGT D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)
RGT K 7732-18-5 Water

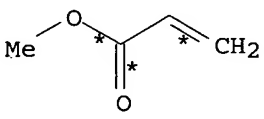
PRO CR 501419-30-3

RX(28) RCT CR 501419-30-3
RGT CT 7664-39-3 HF
PRO CS **501419-31-4**
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

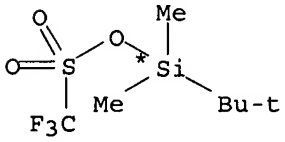
RX(418) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30)
RX(418) U + V + 3 BY + CF + BD + AT + CV ===> **CW**



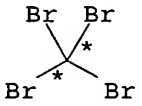
U



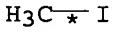
V



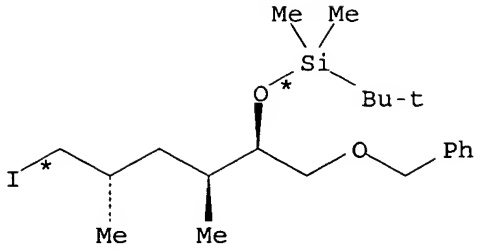
3 BY



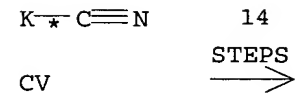
CF



BD

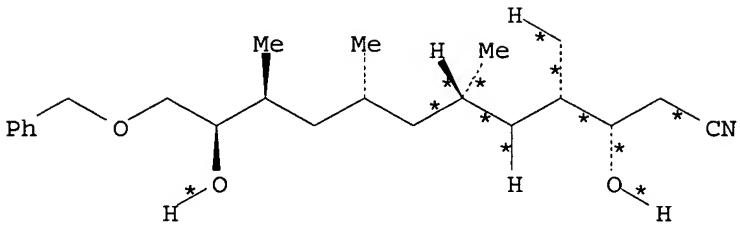


AT



CV

14 STEPS



CW
YIELD 92%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

```
            STAGE(1)
               RGT  CA 108-48-5 2,6-Lutidine
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RCT  BY 69739-34-0
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 15 minutes, 0 deg C
                    SUBSTAGE(2) 0 deg C -> room temperature
                    SUBSTAGE(3) 1 hour, room temperature

            STAGE(3)
               RGT  G 144-55-8 NaHCO3
               SOL  7732-18-5 Water

          PRO  BZ 501419-19-8

RX(17)    RCT  BZ 501419-19-8

            STAGE(1)
               RGT  BF 1191-15-7 AlH(Bu-i)2
               SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 45 minutes, -78 deg C
                    SUBSTAGE(3) 30 minutes, 0 deg C

            STAGE(2)
               RGT  O 67-56-1 MeOH

            STAGE(3)
               RGT  CC 304-59-6 Rochelle salt
               SOL  7732-18-5 Water

          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3
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```
RX(20)     RCT  CG 501419-22-3

             STAGE(1)
                RGT  CH 109-72-8 BuLi
                SOL  109-99-9 THF, 110-54-3 Hexane
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) -78 deg C -> -25 deg C
                     SUBSTAGE(3) 1 hour, -25 deg C
                     SUBSTAGE(4) -25 deg C -> -78 deg C

             STAGE(2)
                RCT  BD 74-88-4
                SOL  109-99-9 THF
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

             STAGE(3)
                RGT  AQ 12125-02-9 NH4Cl
                SOL  7732-18-5 Water

           PRO  AB 501419-23-4

RX(5)      RCT  AB 501419-23-4

             STAGE(1)
                RGT  AD 37342-97-5 Hydrozirconocene Cl
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 2 hours, room temperature
                     SUBSTAGE(2) room temperature -> 0 deg C

             STAGE(2)
                RGT  AE 7553-56-2 I2
                SOL  56-23-5 CCl4
                CON  0 deg C

           PRO  AC 501419-02-9
           NTE  in the dark, regioselective, stereoselective

RX(9)      RCT  AT 501419-06-3

             STAGE(1)
                RGT  AV 7646-85-7 ZnCl2
                SOL  60-29-7 Et2O
                CON  SUBSTAGE(1) room temperature
                     SUBSTAGE(2) room temperature -> -78 deg C

             STAGE(2)
                RGT  AW 594-19-4 t-BuLi
                SOL  110-54-3 Hexane
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 5 minutes, -78 deg C
                     SUBSTAGE(3) 1 hour, room temperature

             STAGE(3)
                RCT  AC 501419-02-9
                CAT  14221-01-3 Pd(PPh3)4
                CON  16 hours, room temperature

             STAGE(4)
```

```
            RGT  K 7732-18-5 Water
            SOL  7732-18-5 Water

         PRO  AU 501419-08-5
         NTE  modified Negishi coupling, stage three in the dark

RX(24)   RCT  AU 501419-08-5
         RGT  CM 429-41-4 Bu4N.F
         PRO  AY 501419-27-8
         SOL  109-99-9 THF
         CON  20 hours, room temperature
         NTE  mol. sieves

RX(10)   RCT  AY 501419-27-8
         RGT  BA 1333-74-0 H2
         PRO  AZ 501419-10-9
         CAT  82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-
              diene][1,4-butanediylbis[diphenylphosphine-κP]]-,
              tetrafluoroborate(1-)
         SOL  75-09-2 CH2Cl2
         CON  SUBSTAGE(1) room temperature
              SUBSTAGE(2) 4 hours, room temperature, 700 psi
         NTE  high pressure, stereoselective

RX(25)   RCT  AZ 501419-10-9, BY 69739-34-0

           STAGE(1)
              RGT  CA 108-48-5 2,6-Lutidine
              SOL  75-09-2 CH2Cl2
              CON  SUBSTAGE(1) room temperature -> 0 deg C
                   SUBSTAGE(2) 5 minutes, 0 deg C
                   SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

           STAGE(2)
              RGT  G 144-55-8 NaHCO3
              SOL  7732-18-5 Water

         PRO  CN 501419-28-9

RX(26)   RCT  CN 501419-28-9

           STAGE(1)
              RGT  CP 84-58-2 DDQ
              SOL  75-09-2 CH2Cl2, 7732-18-5 Water
              CON  1 hour, room temperature, pH 7

           STAGE(2)
              RGT  G 144-55-8 NaHCO3
              SOL  7732-18-5 Water

         PRO  CO 501419-29-0
         NTE  chemoselective, buffered soln.

RX(29)   RCT  CO 501419-29-0

           STAGE(1)
              RGT  CQ 124-63-0 MeSO2Cl, D 121-44-8 Et3N
              SOL  75-09-2 CH2Cl2
              CON  SUBSTAGE(1) room temperature
                   SUBSTAGE(2) room temperature -> 0 deg C
```

SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)
RGT K 7732-18-5 Water

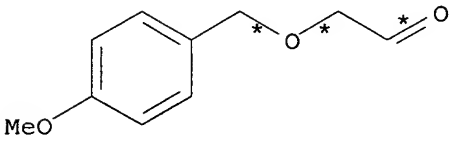
STAGE(3)
RGT CT 7664-39-3 HF
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

STAGE(4)
RGT BJ 584-08-7 K2CO3
SOL 67-56-1 MeOH
CON 45 minutes, room temperature

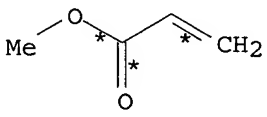
PRO CU 501419-32-5

RX(30) RCT CU 501419-32-5, CV 151-50-8
PRO CW **501419-33-6**
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 70 deg C
SUBSTAGE(3) 24 hours, 70 deg C
SUBSTAGE(4) 70 deg C -> room temperature

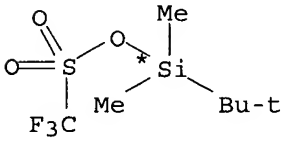
RX(419) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30), RX(31)
RX(419) U + V + 3 BY + CF + BD + AT + CV + 2 CX ===>
BC



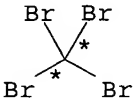
U



V

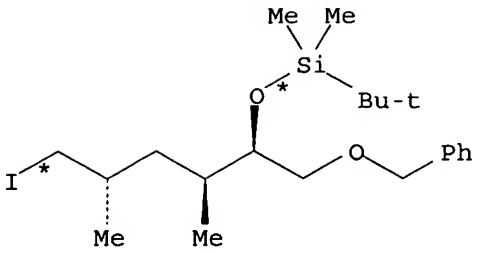


3 BY

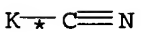


CF

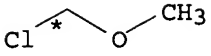
BD



AT

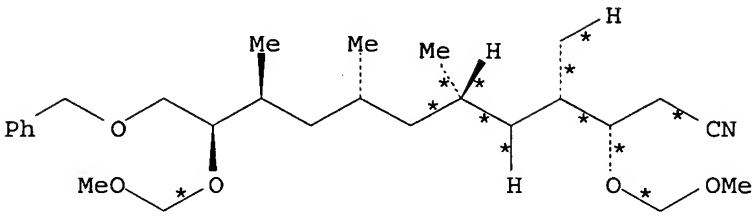


CV



2 CX

15
STEPS



BC
YIELD 81%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

```
          PRO  W 501419-01-8
          NTE  stereoselective

RX(16)    RCT  W 501419-01-8

             STAGE(1)
                RGT  CA 108-48-5 2,6-Lutidine
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) room temperature
                     SUBSTAGE(2) room temperature -> 0 deg C

             STAGE(2)
                RCT  BY 69739-34-0
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 15 minutes, 0 deg C
                     SUBSTAGE(2) 0 deg C -> room temperature
                     SUBSTAGE(3) 1 hour, room temperature

             STAGE(3)
                RGT  G 144-55-8 NaHCO3
                SOL  7732-18-5 Water

          PRO  BZ 501419-19-8

RX(17)    RCT  BZ 501419-19-8

             STAGE(1)
                RGT  BF 1191-15-7 AlH(Bu-i)2
                SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 45 minutes, -78 deg C
                     SUBSTAGE(3) 30 minutes, 0 deg C

             STAGE(2)
                RGT  O 67-56-1 MeOH

             STAGE(3)
                RGT  CC 304-59-6 Rochelle salt
                SOL  7732-18-5 Water

          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

             STAGE(1)
                RGT  AI 603-35-0 PPh3
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 0 deg C
                     SUBSTAGE(2) 0 deg C -> -78 deg C

             STAGE(2)
                RCT  CD 501419-21-2
                SOL  75-09-2 CH2Cl2
```

```
          CON  SUBSTAGE(1) -78 deg C
               SUBSTAGE(2) 30 minutes, -78 deg C
               SUBSTAGE(3) 10 minutes, 0 deg C

     PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

       STAGE(1)
          RGT  CH 109-72-8 BuLi
          SOL  109-99-9 THF, 110-54-3 Hexane
          CON  SUBSTAGE(1) -78 deg C
               SUBSTAGE(2) -78 deg C -> -25 deg C
               SUBSTAGE(3) 1 hour, -25 deg C
               SUBSTAGE(4) -25 deg C -> -78 deg C

       STAGE(2)
          RCT  BD 74-88-4
          SOL  109-99-9 THF
          CON  SUBSTAGE(1) -78 deg C
               SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

       STAGE(3)
          RGT  AQ 12125-02-9 NH4Cl
          SOL  7732-18-5 Water

     PRO  AB 501419-23-4

RX(5)     RCT  AB 501419-23-4

       STAGE(1)
          RGT  AD 37342-97-5 Hydrozirconocene Cl
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) 2 hours, room temperature
               SUBSTAGE(2) room temperature -> 0 deg C

       STAGE(2)
          RGT  AE 7553-56-2 I2
          SOL  56-23-5 CCl4
          CON  0 deg C

     PRO  AC 501419-02-9
     NTE  in the dark, regioselective, stereoselective

RX(9)     RCT  AT 501419-06-3

       STAGE(1)
          RGT  AV 7646-85-7 ZnCl2
          SOL  60-29-7 Et2O
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) room temperature -> -78 deg C

       STAGE(2)
          RGT  AW 594-19-4 t-BuLi
          SOL  110-54-3 Hexane
          CON  SUBSTAGE(1) -78 deg C
               SUBSTAGE(2) 5 minutes, -78 deg C
               SUBSTAGE(3) 1 hour, room temperature

       STAGE(3)
```

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh3)4
CON 16 hours, room temperature

STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu4N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H2
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

STAGE(1)
RGT CQ 124-63-0 MeSO2Cl, D 121-44-8 Et3N
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C
SUBSTAGE(3) 3 minutes, 0 deg C
SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

STAGE(2)
RGT K 7732-18-5 Water

STAGE(3)
RGT CT 7664-39-3 HF
SOL 75-05-8 MeCN, 7732-18-5 Water
CON 3 hours, room temperature

STAGE(4)
RGT BJ 584-08-7 K2CO3
SOL 67-56-1 MeOH
CON 45 minutes, room temperature

PRO CU 501419-32-5

RX(30) RCT CU 501419-32-5, CV 151-50-8
PRO CW 501419-33-6
SOL 75-05-8 MeCN
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 70 deg C
SUBSTAGE(3) 24 hours, 70 deg C
SUBSTAGE(4) 70 deg C -> room temperature

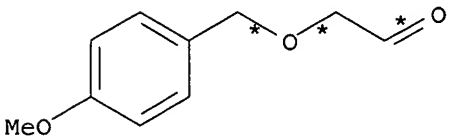
RX(31) RCT CW 501419-33-6, CX 107-30-2

STAGE(1)
RGT CY 7087-68-5 EtN(Pr-i)2
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 28 hours, 0 deg C -> room temperature

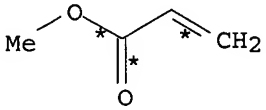
STAGE(2)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO BC **501419-34-7**

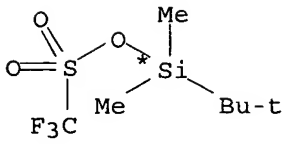
RX(476) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30), RX(31), RX(11)
RX(476) U + V + 3 BY + CF + 2 BD + AT + CV + 2 CX ===>
BE



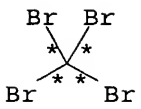
U



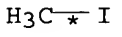
V



3 BY



CF



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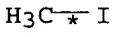

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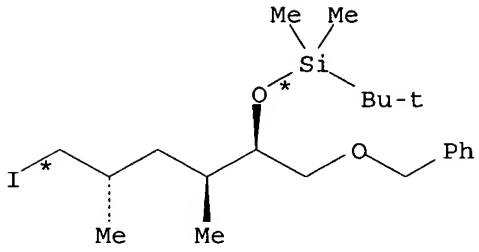
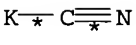
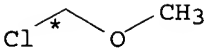


AT

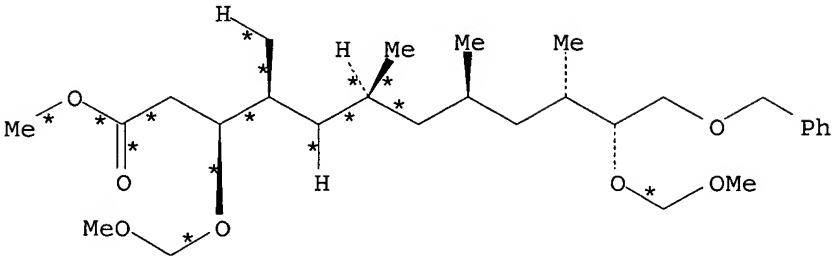


CV



2 CX

16
STEPS



BE
YIELD 88%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)

```
          RGT  X 760-32-7 MeEt2SiH
          SOL  107-06-2 ClCH2CH2Cl
          CON  30 minutes, room temperature

       STAGE(3)
          RCT  U 121289-23-4, V 96-33-3
          SOL  107-06-2 ClCH2CH2Cl
          CON  48 hours, room temperature

       STAGE(4)
          RGT  N 7647-01-0 HCl
          SOL  109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
          CON  30 minutes, room temperature

    PRO   W 501419-01-8
    NTE   stereoselective

RX(16)  RCT   W 501419-01-8

       STAGE(1)
          RGT  CA 108-48-5 2,6-Lutidine
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) room temperature -> 0 deg C

       STAGE(2)
          RCT  BY 69739-34-0
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) 15 minutes, 0 deg C
               SUBSTAGE(2) 0 deg C -> room temperature
               SUBSTAGE(3) 1 hour, room temperature

       STAGE(3)
          RGT  G 144-55-8 NaHCO3
          SOL  7732-18-5 Water

    PRO   BZ 501419-19-8

RX(17)  RCT   BZ 501419-19-8

       STAGE(1)
          RGT  BF 1191-15-7 AlH(Bu-i)2
          SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
          CON  SUBSTAGE(1) -78 deg C
               SUBSTAGE(2) 45 minutes, -78 deg C
               SUBSTAGE(3) 30 minutes, 0 deg C

       STAGE(2)
          RGT  O 67-56-1 MeOH

       STAGE(3)
          RGT  CC 304-59-6 Rochelle salt
          SOL  7732-18-5 Water

    PRO   CB 501419-20-1

RX(18)  RCT   CB 501419-20-1
    RGT   CE 87413-09-0 Martin's reagent
    PRO   CD 501419-21-2
    SOL   75-09-2 CH2Cl2
```

```
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

             STAGE(1)
                RGT  AI 603-35-0 PPh3
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 0 deg C
                     SUBSTAGE(2) 0 deg C -> -78 deg C

             STAGE(2)
                RCT  CD 501419-21-2
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 30 minutes, -78 deg C
                     SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

             STAGE(1)
                RGT  CH 109-72-8 BuLi
                SOL  109-99-9 THF, 110-54-3 Hexane
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) -78 deg C -> -25 deg C
                     SUBSTAGE(3) 1 hour, -25 deg C
                     SUBSTAGE(4) -25 deg C -> -78 deg C

             STAGE(2)
                RCT  BD 74-88-4
                SOL  109-99-9 THF
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

             STAGE(3)
                RGT  AQ 12125-02-9 NH4Cl
                SOL  7732-18-5 Water

          PRO  AB 501419-23-4

RX(5)     RCT  AB 501419-23-4

             STAGE(1)
                RGT  AD 37342-97-5 Hydrozirconocene Cl
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 2 hours, room temperature
                     SUBSTAGE(2) room temperature -> 0 deg C

             STAGE(2)
                RGT  AE 7553-56-2 I2
                SOL  56-23-5 CCl4
                CON  0 deg C

          PRO  AC 501419-02-9
          NTE  in the dark, regioselective, stereoselective

RX(9)     RCT  AT 501419-06-3

             STAGE(1)
```

```
            RGT  AV 7646-85-7 ZnCl2
            SOL  60-29-7 Et2O
            CON  SUBSTAGE(1) room temperature
                 SUBSTAGE(2) room temperature -> -78 deg C

         STAGE(2)
            RGT  AW 594-19-4 t-BuLi
            SOL  110-54-3 Hexane
            CON  SUBSTAGE(1) -78 deg C
                 SUBSTAGE(2) 5 minutes, -78 deg C
                 SUBSTAGE(3) 1 hour, room temperature

         STAGE(3)
            RCT  AC 501419-02-9
            CAT  14221-01-3 Pd(PPh3)4
            CON  16 hours, room temperature

         STAGE(4)
            RGT  K 7732-18-5 Water
            SOL  7732-18-5 Water

      PRO  AU 501419-08-5
      NTE  modified Negishi coupling, stage three in the dark

RX(24)   RCT  AU 501419-08-5
         RGT  CM 429-41-4 Bu4N.F
         PRO  AY 501419-27-8
         SOL  109-99-9 THF
         CON  20 hours, room temperature
         NTE  mol. sieves

RX(10)   RCT  AY 501419-27-8
         RGT  BA 1333-74-0 H2
         PRO  AZ 501419-10-9
         CAT  82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-
              diene][1,4-butanediylbis[diphenylphosphine-κP]]-,
              tetrafluoroborate(1-)
         SOL  75-09-2 CH2Cl2
         CON  SUBSTAGE(1) room temperature
              SUBSTAGE(2) 4 hours, room temperature, 700 psi
         NTE  high pressure, stereoselective

RX(25)   RCT  AZ 501419-10-9, BY 69739-34-0

         STAGE(1)
            RGT  CA 108-48-5 2,6-Lutidine
            SOL  75-09-2 CH2Cl2
            CON  SUBSTAGE(1) room temperature -> 0 deg C
                 SUBSTAGE(2) 5 minutes, 0 deg C
                 SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

         STAGE(2)
            RGT  G 144-55-8 NaHCO3
            SOL  7732-18-5 Water

      PRO  CN 501419-28-9

RX(26)   RCT  CN 501419-28-9

         STAGE(1)
```

```
                RGT  CP 84-58-2 DDQ
                SOL  75-09-2 CH2Cl2, 7732-18-5 Water
                CON  1 hour, room temperature, pH 7

             STAGE(2)
                RGT  G 144-55-8 NaHCO3
                SOL  7732-18-5 Water

          PRO  CO 501419-29-0
          NTE  chemoselective, buffered soln.

RX(29)    RCT  CO 501419-29-0

             STAGE(1)
                RGT  CQ 124-63-0 MeSO2Cl, D 121-44-8 Et3N
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) room temperature
                     SUBSTAGE(2) room temperature -> 0 deg C
                     SUBSTAGE(3) 3 minutes, 0 deg C
                     SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

             STAGE(2)
                RGT  K 7732-18-5 Water

             STAGE(3)
                RGT  CT 7664-39-3 HF
                SOL  75-05-8 MeCN, 7732-18-5 Water
                CON  3 hours, room temperature

             STAGE(4)
                RGT  BJ 584-08-7 K2CO3
                SOL  67-56-1 MeOH
                CON  45 minutes, room temperature

          PRO  CU 501419-32-5

RX(30)    RCT  CU 501419-32-5, CV 151-50-8
          PRO  CW 501419-33-6
          SOL  75-05-8 MeCN
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) room temperature -> 70 deg C
               SUBSTAGE(3) 24 hours, 70 deg C
               SUBSTAGE(4) 70 deg C -> room temperature

RX(31)    RCT  CW 501419-33-6, CX 107-30-2

             STAGE(1)
                RGT  CY 7087-68-5 EtN(Pr-i)2
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 0 deg C
                     SUBSTAGE(2) 28 hours, 0 deg C -> room temperature

             STAGE(2)
                RGT  K 7732-18-5 Water
                SOL  7732-18-5 Water

          PRO  BC 501419-34-7

RX(11)    RCT  BC 501419-34-7
```

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON 1 hour, -78 deg C

STAGE(2)
RGT N 7647-01-0 HCl
SOL 7732-18-5 Water
CON SUBSTAGE(2) 20 minutes, room temperature

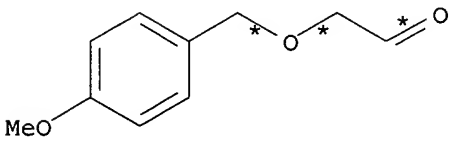
STAGE(3)
RGT BG 513-35-9 Me2C:CHMe, BH 7758-19-2 NaOClO, BI 7558-80-7 NaH2PO4
SOL 75-65-0 t-BuOH, 7732-18-5 Water
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 1 hour, 0 deg C

STAGE(4)
RCT BD 74-88-4
RGT BJ 584-08-7 K2CO3
SOL 68-12-2 DMF
CON 3.5 hours, room temperature

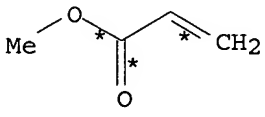
PRO BE **501419-14-3**

RX(477) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25), RX(26), RX(29), RX(30), RX(31), RX(32)

RX(477) U + V + 3 BY + CF + BD + AT + CV + 2 CX ===> **CZ**



U



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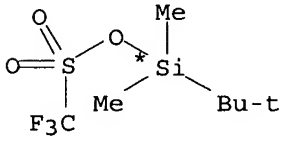
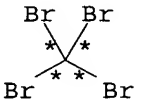
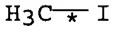


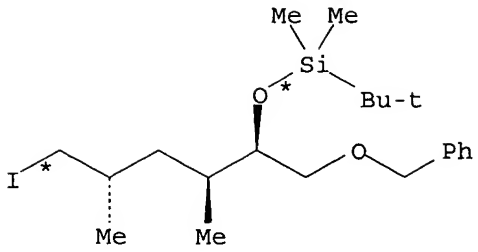
3 BY



CF



BD



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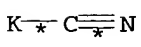

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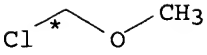
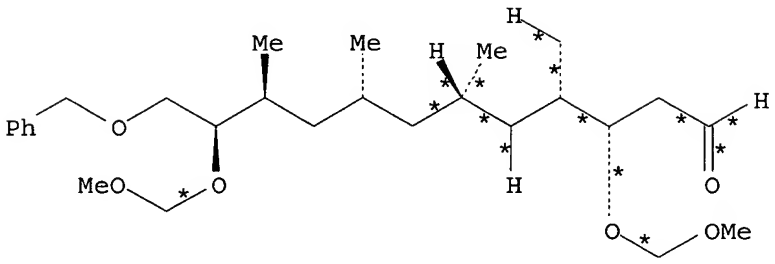


2 CX

16
STEPS



CZ

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

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          PRO  W 501419-01-8
          NTE  stereoselective

RX(16)    RCT  W 501419-01-8

             STAGE(1)
                RGT  CA 108-48-5 2,6-Lutidine
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) room temperature
                     SUBSTAGE(2) room temperature -> 0 deg C

             STAGE(2)
                RCT  BY 69739-34-0
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 15 minutes, 0 deg C
                     SUBSTAGE(2) 0 deg C -> room temperature
                     SUBSTAGE(3) 1 hour, room temperature

             STAGE(3)
                RGT  G 144-55-8 NaHCO3
                SOL  7732-18-5 Water

          PRO  BZ 501419-19-8

RX(17)    RCT  BZ 501419-19-8

             STAGE(1)
                RGT  BF 1191-15-7 AlH(Bu-i)2
                SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
                CON  SUBSTAGE(1) -78 deg C
                     SUBSTAGE(2) 45 minutes, -78 deg C
                     SUBSTAGE(3) 30 minutes, 0 deg C

             STAGE(2)
                RGT  O 67-56-1 MeOH

             STAGE(3)
                RGT  CC 304-59-6 Rochelle salt
                SOL  7732-18-5 Water

          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

             STAGE(1)
                RGT  AI 603-35-0 PPh3
                SOL  75-09-2 CH2Cl2
                CON  SUBSTAGE(1) 0 deg C
                     SUBSTAGE(2) 0 deg C -> -78 deg C

             STAGE(2)
                RCT  CD 501419-21-2
                SOL  75-09-2 CH2Cl2
```

```
            CON  SUBSTAGE(1) -78 deg C
                 SUBSTAGE(2) 30 minutes, -78 deg C
                 SUBSTAGE(3) 10 minutes, 0 deg C

         PRO  CG 501419-22-3

RX(20)   RCT  CG 501419-22-3

           STAGE(1)
              RGT  CH 109-72-8 BuLi
              SOL  109-99-9 THF, 110-54-3 Hexane
              CON  SUBSTAGE(1) -78 deg C
                   SUBSTAGE(2) -78 deg C -> -25 deg C
                   SUBSTAGE(3) 1 hour, -25 deg C
                   SUBSTAGE(4) -25 deg C -> -78 deg C

           STAGE(2)
              RCT  BD 74-88-4
              SOL  109-99-9 THF
              CON  SUBSTAGE(1) -78 deg C
                   SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

           STAGE(3)
              RGT  AQ 12125-02-9 NH4Cl
              SOL  7732-18-5 Water

         PRO  AB 501419-23-4

RX(5)    RCT  AB 501419-23-4

           STAGE(1)
              RGT  AD 37342-97-5 Hydrozirconocene Cl
              SOL  75-09-2 CH2Cl2
              CON  SUBSTAGE(1) 2 hours, room temperature
                   SUBSTAGE(2) room temperature -> 0 deg C

           STAGE(2)
              RGT  AE 7553-56-2 I2
              SOL  56-23-5 CCl4
              CON  0 deg C

         PRO  AC 501419-02-9
         NTE  in the dark, regioselective, stereoselective

RX(9)    RCT  AT 501419-06-3

           STAGE(1)
              RGT  AV 7646-85-7 ZnCl2
              SOL  60-29-7 Et2O
              CON  SUBSTAGE(1) room temperature
                   SUBSTAGE(2) room temperature -> -78 deg C

           STAGE(2)
              RGT  AW 594-19-4 t-BuLi
              SOL  110-54-3 Hexane
              CON  SUBSTAGE(1) -78 deg C
                   SUBSTAGE(2) 5 minutes, -78 deg C
                   SUBSTAGE(3) 1 hour, room temperature

           STAGE(3)
```

RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh3)4
CON 16 hours, room temperature

STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu4N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H2
PRO AZ 501419-10-9
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(25) RCT AZ 501419-10-9, BY 69739-34-0

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 5 minutes, 0 deg C
SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CN 501419-28-9

RX(26) RCT CN 501419-28-9

STAGE(1)
RGT CP 84-58-2 DDQ
SOL 75-09-2 CH2Cl2, 7732-18-5 Water
CON 1 hour, room temperature, pH 7

STAGE(2)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO CO 501419-29-0
NTE chemoselective, buffered soln.

RX(29) RCT CO 501419-29-0

```
            STAGE(1)
               RGT  CQ 124-63-0 MeSO2Cl, D 121-44-8 Et3N
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C
                    SUBSTAGE(3) 3 minutes, 0 deg C
                    SUBSTAGE(4) 1.5 hours, 0 deg C -> room temperature

            STAGE(2)
               RGT  K 7732-18-5 Water

            STAGE(3)
               RGT  CT 7664-39-3 HF
               SOL  75-05-8 MeCN, 7732-18-5 Water
               CON  3 hours, room temperature

            STAGE(4)
               RGT  BJ 584-08-7 K2CO3
               SOL  67-56-1 MeOH
               CON  45 minutes, room temperature

         PRO  CU 501419-32-5

RX(30)   RCT  CU 501419-32-5, CV 151-50-8
         PRO  CW 501419-33-6
         SOL  75-05-8 MeCN
         CON  SUBSTAGE(1) room temperature
              SUBSTAGE(2) room temperature -> 70 deg C
              SUBSTAGE(3) 24 hours, 70 deg C
              SUBSTAGE(4) 70 deg C -> room temperature

RX(31)   RCT  CW 501419-33-6, CX 107-30-2

            STAGE(1)
               RGT  CY 7087-68-5 EtN(Pr-i)2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 28 hours, 0 deg C -> room temperature

            STAGE(2)
               RGT  K 7732-18-5 Water
               SOL  7732-18-5 Water

         PRO  BC 501419-34-7

RX(32)   RCT  BC 501419-34-7

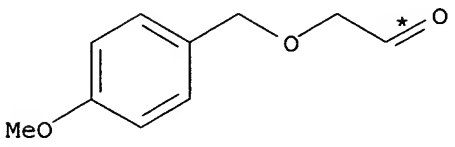
            STAGE(1)
               RGT  BF 1191-15-7 AlH(Bu-i)2
               SOL  75-09-2 CH2Cl2, 110-54-3 Hexane
               CON  1 hour, -78 deg C

            STAGE(2)
               RGT  N 7647-01-0 HCl
               SOL  7732-18-5 Water
               CON  SUBSTAGE(2) 20 minutes, room temperature

         PRO  CZ 501419-35-8
```

RX(555) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10)

RX(555) U + V + BY + CF + BD + AT ===> **AZ**



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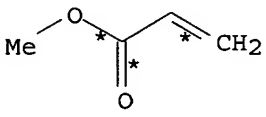

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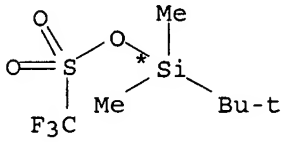
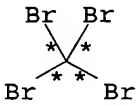


BY



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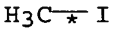

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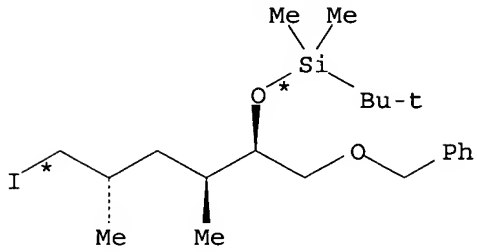
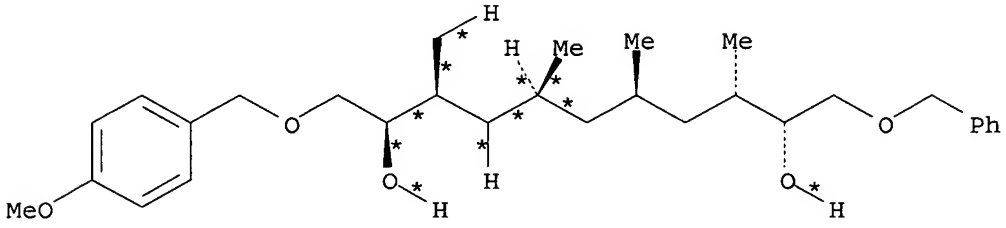


AT

10 STEPS



AZ
YIELD 86%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3**

Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

```
          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

            STAGE(3)
               RGT  AQ 12125-02-9 NH4Cl
               SOL  7732-18-5 Water

          PRO  AB 501419-23-4

RX(5)     RCT  AB 501419-23-4

            STAGE(1)
               RGT  AD 37342-97-5 Hydrozirconocene Cl
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 2 hours, room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RGT  AE 7553-56-2 I2
               SOL  56-23-5 CCl4
               CON  0 deg C
```

PRO AC 501419-02-9
NTE in the dark, regioselective, stereoselective

RX(9) RCT AT 501419-06-3

STAGE(1)
RGT AV 7646-85-7 ZnCl2
SOL 60-29-7 Et2O
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> -78 deg C

STAGE(2)
RGT AW 594-19-4 t-BuLi
SOL 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 5 minutes, -78 deg C
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RCT AC 501419-02-9
CAT 14221-01-3 Pd(PPh3)4
CON 16 hours, room temperature

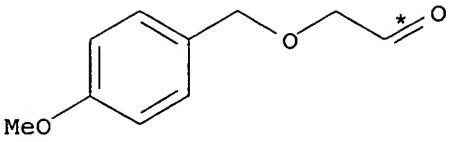
STAGE(4)
RGT K 7732-18-5 Water
SOL 7732-18-5 Water

PRO AU 501419-08-5
NTE modified Negishi coupling, stage three in the dark

RX(24) RCT AU 501419-08-5
RGT CM 429-41-4 Bu4N.F
PRO AY 501419-27-8
SOL 109-99-9 THF
CON 20 hours, room temperature
NTE mol. sieves

RX(10) RCT AY 501419-27-8
RGT BA 1333-74-0 H2
PRO AZ **501419-10-9**
CAT 82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene][1,4-butanediylbis[diphenylphosphine-κP]]-, tetrafluoroborate(1-)
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 4 hours, room temperature, 700 psi
NTE high pressure, stereoselective

RX(558) OF 594 COMPOSED OF RX(4), RX(16), RX(17), RX(18), RX(19), RX(20), RX(5), RX(9), RX(24), RX(10), RX(25)
RX(558) U + V + 3 BY + CF + BD + AT ===> **CN**



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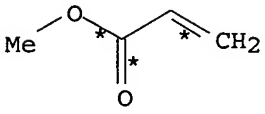

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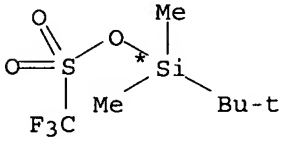

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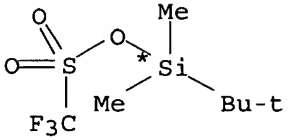
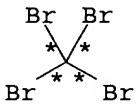


2 BY



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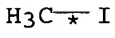

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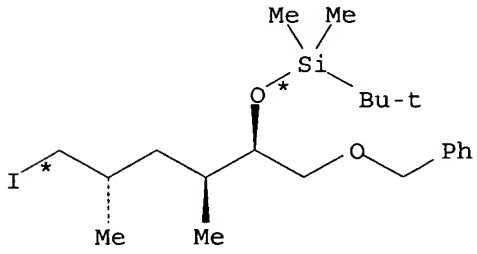
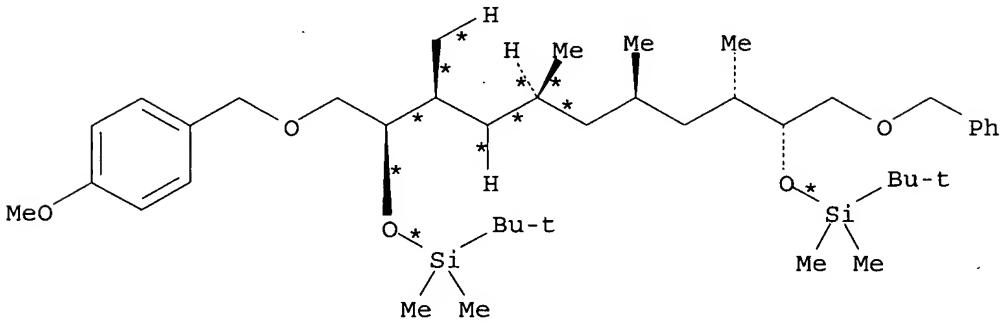


AT

11
STEPS



CN
YIELD 100%

RX(4)

STAGE(1)
CAT 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-

[2(3aR*,8aS*),3aα,8aα]]-, **12112-67-3**
Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 107-06-2 ClCH2CH2Cl
CON 1 hour, room temperature

STAGE(2)
RGT X **760-32-7** MeEt2SiH
SOL 107-06-2 ClCH2CH2Cl
CON 30 minutes, room temperature

STAGE(3)
RCT U 121289-23-4, V 96-33-3
SOL 107-06-2 ClCH2CH2Cl
CON 48 hours, room temperature

STAGE(4)
RGT N 7647-01-0 HCl
SOL 109-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water
CON 30 minutes, room temperature

PRO W 501419-01-8
NTE stereoselective

RX(16) RCT W 501419-01-8

STAGE(1)
RGT CA 108-48-5 2,6-Lutidine
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature -> 0 deg C

STAGE(2)
RCT BY 69739-34-0
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 15 minutes, 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 1 hour, room temperature

STAGE(3)
RGT G 144-55-8 NaHCO3
SOL 7732-18-5 Water

PRO BZ 501419-19-8

RX(17) RCT BZ 501419-19-8

STAGE(1)
RGT BF 1191-15-7 AlH(Bu-i)2
SOL 75-09-2 CH2Cl2, 110-54-3 Hexane
CON SUBSTAGE(1) -78 deg C
SUBSTAGE(2) 45 minutes, -78 deg C
SUBSTAGE(3) 30 minutes, 0 deg C

STAGE(2)
RGT O 67-56-1 MeOH

STAGE(3)
RGT CC 304-59-6 Rochelle salt
SOL 7732-18-5 Water

```
          PRO  CB 501419-20-1

RX(18)    RCT  CB 501419-20-1
          RGT  CE 87413-09-0 Martin's reagent
          PRO  CD 501419-21-2
          SOL  75-09-2 CH2Cl2
          CON  90 minutes, room temperature

RX(19)    RCT  CF 558-13-4

            STAGE(1)
               RGT  AI 603-35-0 PPh3
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0 deg C
                    SUBSTAGE(2) 0 deg C -> -78 deg C

            STAGE(2)
               RCT  CD 501419-21-2
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 30 minutes, -78 deg C
                    SUBSTAGE(3) 10 minutes, 0 deg C

          PRO  CG 501419-22-3

RX(20)    RCT  CG 501419-22-3

            STAGE(1)
               RGT  CH 109-72-8 BuLi
               SOL  109-99-9 THF, 110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) -78 deg C -> -25 deg C
                    SUBSTAGE(3) 1 hour, -25 deg C
                    SUBSTAGE(4) -25 deg C -> -78 deg C

            STAGE(2)
               RCT  BD 74-88-4
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 1 hour, -78 deg C -> room temperature

            STAGE(3)
               RGT  AQ 12125-02-9 NH4Cl
               SOL  7732-18-5 Water

          PRO  AB 501419-23-4

RX(5)     RCT  AB 501419-23-4

            STAGE(1)
               RGT  AD 37342-97-5 Hydrozirconocene Cl
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 2 hours, room temperature
                    SUBSTAGE(2) room temperature -> 0 deg C

            STAGE(2)
               RGT  AE 7553-56-2 I2
               SOL  56-23-5 CCl4
               CON  0 deg C
```

```
          PRO  AC 501419-02-9
          NTE  in the dark, regioselective, stereoselective

RX(9)     RCT  AT 501419-06-3

            STAGE(1)
               RGT  AV 7646-85-7 ZnCl2
               SOL  60-29-7 Et2O
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) room temperature -> -78 deg C

            STAGE(2)
               RGT  AW 594-19-4 t-BuLi
               SOL  110-54-3 Hexane
               CON  SUBSTAGE(1) -78 deg C
                    SUBSTAGE(2) 5 minutes, -78 deg C
                    SUBSTAGE(3) 1 hour, room temperature

            STAGE(3)
               RCT  AC 501419-02-9
               CAT  14221-01-3 Pd(PPh3)4
               CON  16 hours, room temperature

            STAGE(4)
               RGT  K 7732-18-5 Water
               SOL  7732-18-5 Water

          PRO  AU 501419-08-5
          NTE  modified Negishi coupling, stage three in the dark

RX(24)    RCT  AU 501419-08-5
          RGT  CM 429-41-4 Bu4N.F
          PRO  AY 501419-27-8
          SOL  109-99-9 THF
          CON  20 hours, room temperature
          NTE  mol. sieves

RX(10)    RCT  AY 501419-27-8
          RGT  BA 1333-74-0 H2
          PRO  AZ 501419-10-9
          CAT  82499-43-2 Rhodium(1+), [(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-
               diene][1,4-butanediylbis[diphenylphosphine-κP]]-,
               tetrafluoroborate(1-)
          SOL  75-09-2 CH2Cl2
          CON  SUBSTAGE(1) room temperature
               SUBSTAGE(2) 4 hours, room temperature, 700 psi
          NTE  high pressure, stereoselective

RX(25)    RCT  AZ 501419-10-9, BY 69739-34-0

            STAGE(1)
               RGT  CA 108-48-5 2,6-Lutidine
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) room temperature -> 0 deg C
                    SUBSTAGE(2) 5 minutes, 0 deg C
                    SUBSTAGE(3) 1 hour, 0 deg C -> room temperature

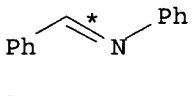
            STAGE(2)
               RGT  G 144-55-8 NaHCO3
```

SOL 7732-18-5 Water

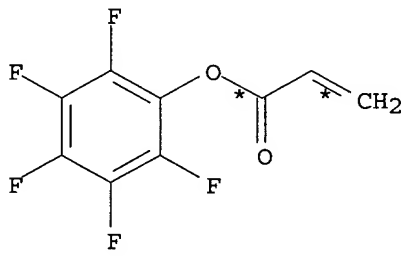
PRO CN **501419-28-9**

L64 ANSWER 19 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 137:185334 CASREACT
TITLE: Stereoselective Synthesis of trans β-Lactams through Iridium-Catalyzed Reductive Coupling of Imines and Acrylates
AUTHOR(S): Townes, Jennifer A.; Evans, Michael A.; Queffelec, Jerome; Taylor, Steven J.; Morken, James P.
CORPORATE SOURCE: Department of Chemistry, Venable and Kenan Laboratories, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290, USA
SOURCE: Organic Letters (2002), 4(15), 2537-2540
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Iridium-catalyzed reductive coupling of acrylates and imines provides trans β-lactams with high diastereoselection. The optimal catalyst allows for the synthesis of trans β-lactams bearing aromatic, alkenyl, and alkynyl side chains. This reaction appears to proceed through a reductive Mannich addition-cyclization mechanism. Examination of substituent effects reveals a linear Hammett correlation for both the N-aryl group on the imine and the aryloxy group on the acrylate, thereby pointing to rate-determining cyclization in the reaction mechanism.
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 8 A + H ===> **C**



A



H

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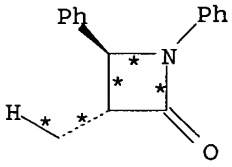
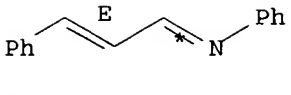


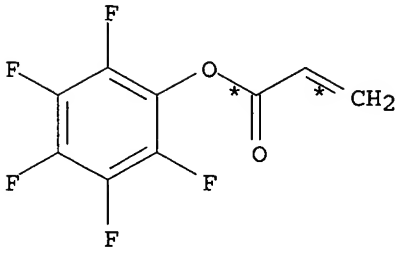
C
YIELD 68%

RX(2) RCT A 538-51-2, H 71195-85-2
RGT D **760-32-7** MeEt2SiH
PRO C **17324-17-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl
NTE stereoselective, optimization study, optimized on metal catalyst/ligand/silane

RX(3) OF 8 K + H ===> **L**



K



H

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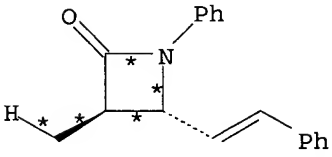
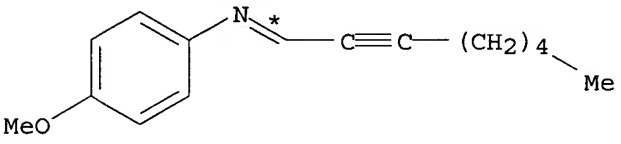


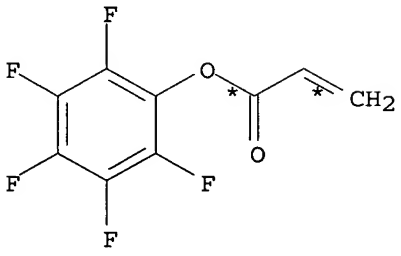
L
YIELD 70%

RX(3) RCT K 52944-37-3, H 71195-85-2
RGT D **760-32-7** MeEt2SiH
PRO L **451455-41-7**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl
NTE stereoselective

RX(4) OF 8 M + H ===> **N**



M



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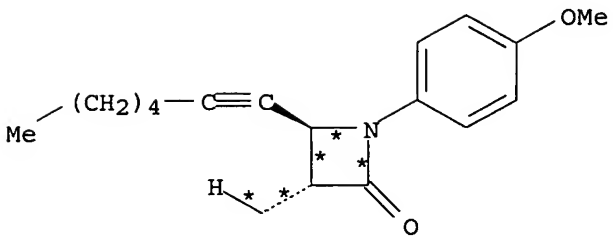
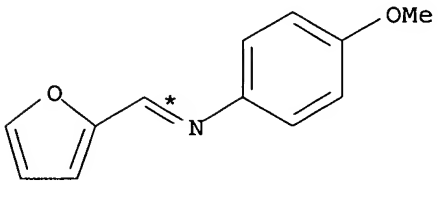


N
YIELD 58%

RX(4) RCT M 451455-39-3, H 71195-85-2
RGT D **760-32-7** MeEt2SiH
PRO N **451455-42-8**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl
NTE stereoselective

RX(5) OF 8 O + H ===> **P**



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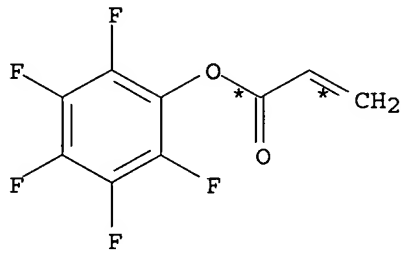

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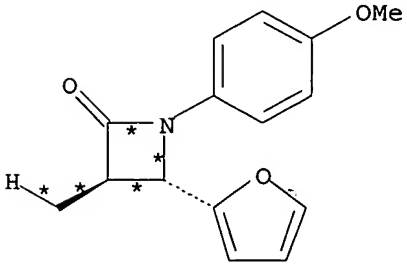
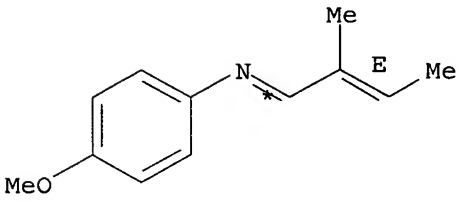


P
YIELD 78%

RX(5) RCT O 1749-14-0, H 71195-85-2
RGT D **760-32-7** MeEt2SiH

PRO P **152899-73-5**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl
NTE stereoselective

RX(6) OF 8 Q + H ===> **R**



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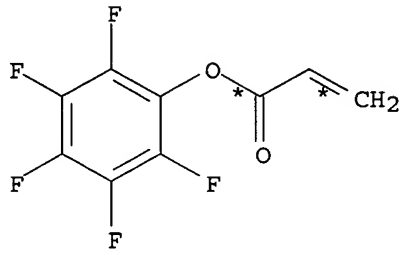

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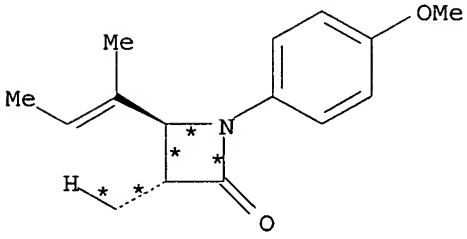
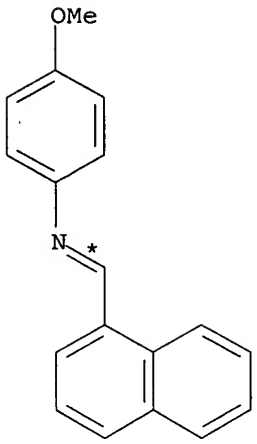


R
YIELD 60%

RX(6) RCT Q 451455-40-6, H 71195-85-2
RGT D **760-32-7** MeEt2SiH
PRO R **451455-43-9**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl
NTE stereoselective

RX(7) OF 8 S + H ===> **T**



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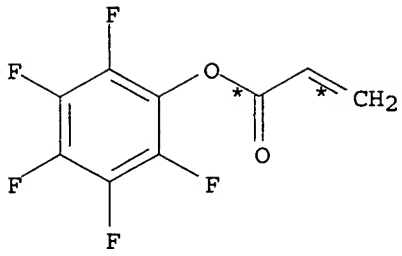

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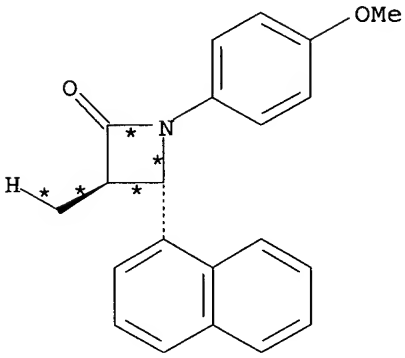
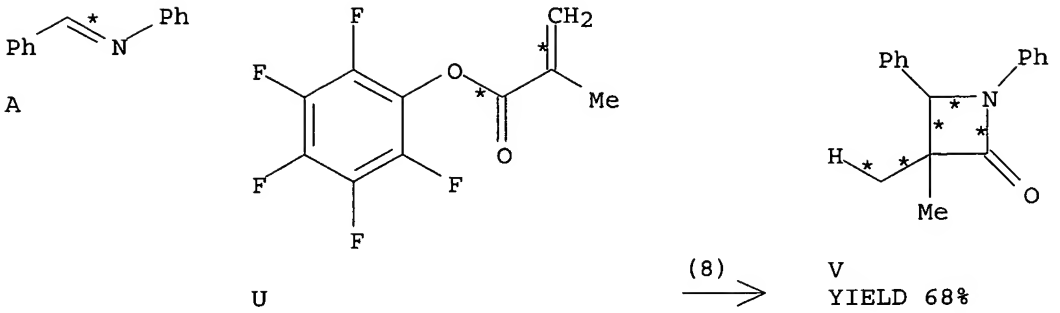


T
YIELD 80%

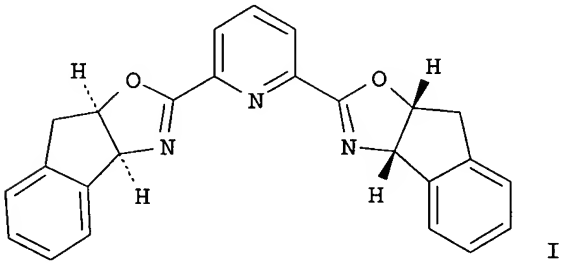
RX(7) RCT S 3525-60-8, H 71195-85-2
RGT D **760-32-7** MeEt2SiH
PRO T **451455-44-0**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl
NTE stereoselective

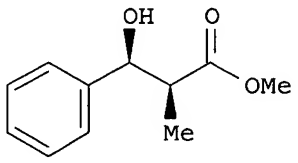
RX(8) OF 8 A + U ===> **V**



RX(8) RCT A 538-51-2, U 13642-97-2
RGT D **760-32-7** MeEt2SiH
PRO V **5438-81-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 101-02-0 P(OPh)3
SOL 107-06-2 ClCH2CH2Cl

L64 ANSWER 20 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 135:107055 CASREACT
TITLE: Enantio- and diastereoselective reductive aldol reactions with iridium-pybox catalysts
AUTHOR(S): Zhao, Cun-Xiang; Duffey, Matthew O.; Taylor, Steven J.; Morken, James P.
CORPORATE SOURCE: Department of Chemistry Venable and Kenan Laboratories, The University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290, USA
SOURCE: Organic Letters (2001), 3(12), 1829-1831
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI


I

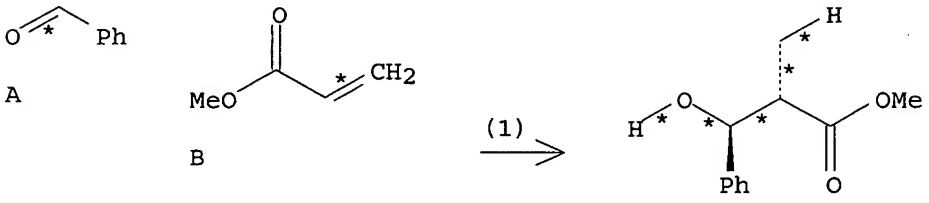

II

AB A catalytic amount of [(COD)IrCl]2 and indane-pybox I converts diethylmethylsilane, Me acrylate, and certain aldehydes to the derived

reductive aldol adduct with good enantio- and diastereocontrol. Thus, reaction of PhCHO with H2C:CHCO2Me and Et2SiHMe in CH2Cl2 containing [(COD)IrCl]2 and I at 25° for 24 h gave the hydroxybenzenepropanoate II in 68% yield with 6.6:1 syn:anti ratio and 97:3 enantiomeric ratio.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 7 A + B ===> **C**



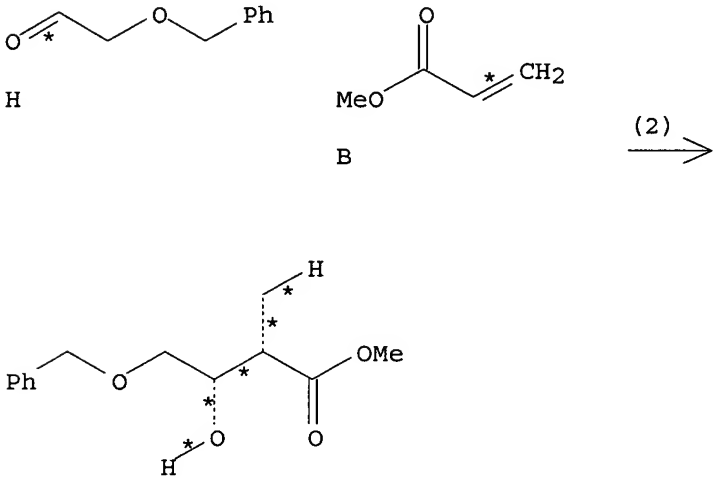
A

B

C
YIELD 68%

RX(1) RCT A 100-52-7, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO C **76549-03-6**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(2) OF 7 H + B ===> **I**



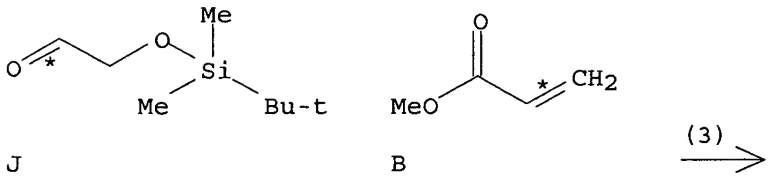
H

B

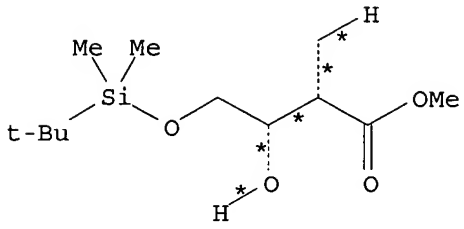
I
YIELD 59%

RX(2) RCT H 60656-87-3, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO I **350256-93-8**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(3) OF 7 J + B ===> **K**



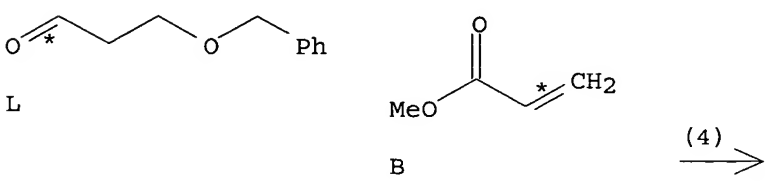
J B (3) ⟶



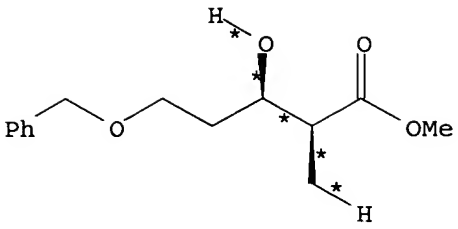
K
YIELD 47%

RX(3) RCT J 102191-92-4, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO K **350256-94-9**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(4) OF 7 L + B ===> **M**



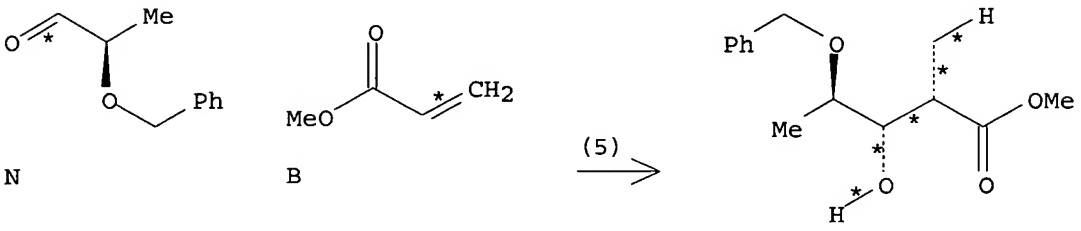
L B (4) ⟶



M
YIELD 65%

RX(4) RCT L 19790-60-4, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO M **350256-95-0**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(5) OF 7 N + B ===> **O**

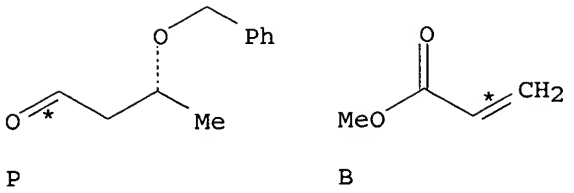


N B O

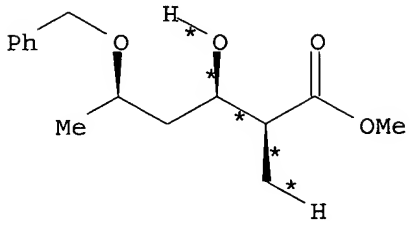
YIELD 50%

RX(5) RCT N 81445-45-6, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO O **350256-96-1**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(6) OF 7 P + B ===> **Q**



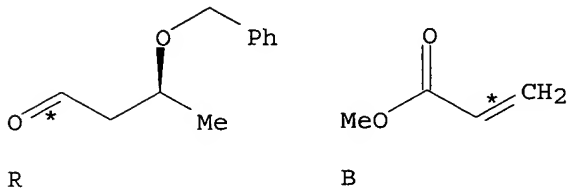
P B (6)



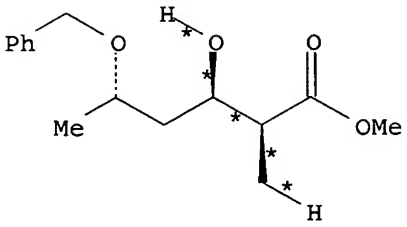
Q
YIELD 65%

RX(6) RCT P 86040-07-5, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO Q **350256-97-2**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

RX(7) OF 7 R + B ===> **S**



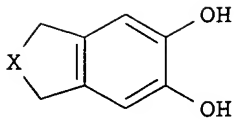
R B (7)



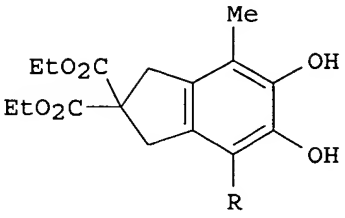
S
YIELD 57%

RX(7) RCT R 99032-03-8, B 96-33-3
RGT D **760-32-7** MeEt2SiH
PRO S **350256-98-3**
CAT **12112-67-3** Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 185346-09-2 8H-Indeno[1,2-d]oxazole, 2,2'-(2,6-pyridinediyl)bis[3a,8a-dihydro-, [3aS-[2(3aR*,8aS*),3aα,8aα]]-
SOL 75-09-2 CH2Cl2
NTE stereoselective

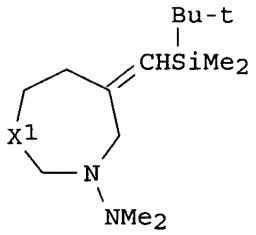
L64 ANSWER 21 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 129:67445 CASREACT
TITLE: Development of novel catalytic systems based on transition metal complexes
AUTHOR(S): Murai, Shinji
CORPORATE SOURCE: Japan
SOURCE: Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku [Electronic Publication] (1996) No pp. Given
CODEN: AGSHEN; ISSN: 0919-9179
PUBLISHER: Asahi Garasu Zaidan
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: Japanese
GI



I



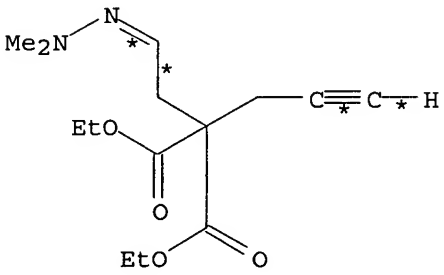
II



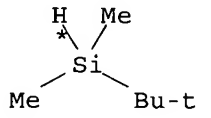
III

AB The reaction of 1,6-diynes HC.tplbond.CCH2XCH2C.tplbond.CH [X = C(CO2Et)2, CH2, O, NTs, S] or MeC.tplbond.CCH2C(CO2Et)2CH2C.tplbond.CR (R = H, Me) with H2O and CO (50 atm) in the presence of Ru3(CO)12 at 140°C in dioxane resulted in the incorporation of two mols. of CO to give catechol derivs. (I; X = same as above) or (II; R = H, Me) in good yields (58-83%). The reaction involves the intermediary of an oxycarbyne complex as a key catalytic species and is the new mode of successive incorporation of two mols. of CO into diynes. The reaction of acetylene-hydrazones HC.tplbond.CCH2X1CH2CH:NNMe2 [X1 = C(CO2Et)2, CH2, bond] with HSiMe2But and CO (10 atm) in the presence of Ir4(CO)12 at 140°C in CH3CN gave 6- or 7-membered nitrogen heterocycles (III; X1 = same as above) having a (trimethylsilyl)methylene group at 3-position. The reaction involves cyclization with incorporation of one mol. of CO and reduction of the incorporated CO carbon to methylene group. The reaction provides a new method for the construction of nitrogen heterocycles. Thus, reaction of HC.tplbond.CCH2C(CO2Et)2CH2C.tplbond.CH with H2O and CO in the presence of Ru3(CO)12 in dioxane at 50 atm and 140° gave 83% I [X = C(CO2Et)2].

RX(7) OF 7 Q + **R** + B ===> **S**



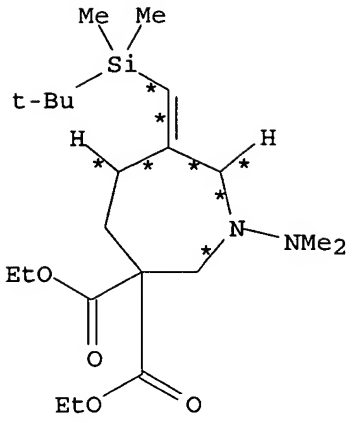
Q



R

B

(7) ⟶

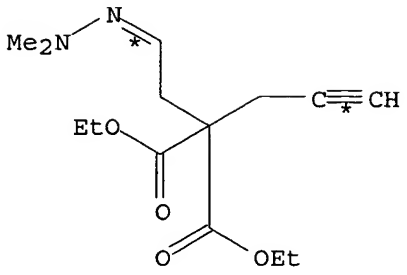


S
YIELD 53%

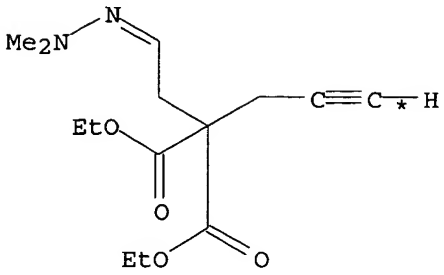
RX(7) RCT Q 168557-46-8, R **29681-57-0**, B 630-08-0
PRO S **208830-57-3**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE 10 atm and 140°

L64 ANSWER 22 OF 38 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 123:228275 CASREACT
TITLE: Iridium-Catalyzed Reaction of Acetylene Hydrazones with a Hydrosilane and Carbon Monoxide. Synthesis of Nitrogen Heterocycles
AUTHOR(S): Chatani, Naoto; Yamaguchi, Shinshi; Fukumoto, Yoshiya; Murai, Shinji
CORPORATE SOURCE: Faculty of Engineering, Osaka University, Suita, 565, Japan
SOURCE: Organometallics (1995), 14(9), 4418-20
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction of acetylene hydrazones with a hydrosilane and carbon monoxide (CO) in the presence of Ir4(CO)12 as the catalyst gave six- or seven-membered nitrogen heterocycles having a (tert-butyldimethylsilyl)methylene group at the 3-position.

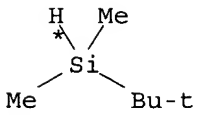
RX(2) OF 16 ...2 D + 2 **F** + G ===> **H** + **I**



D



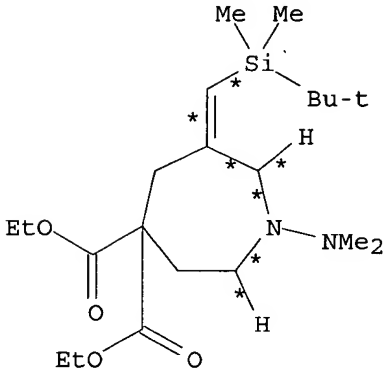
D



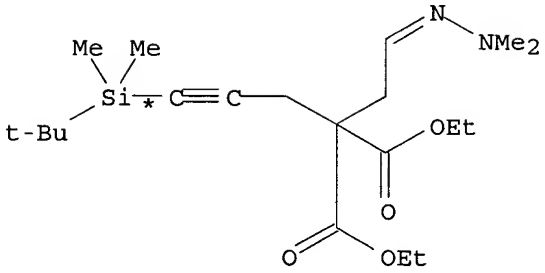
2 F

G

(2) ⟶



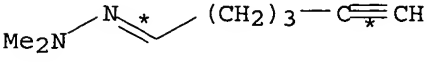
H
YIELD 53%



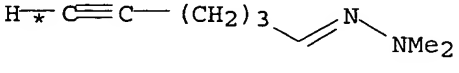
I
YIELD 8%

RX(2) RCT D 168557-46-8, F **29681-57-0**, G 630-08-0
PRO H **168557-47-9**, I **168557-48-0**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure, optimization study, optimized on reaction temperature,pressure of CO,catalyst

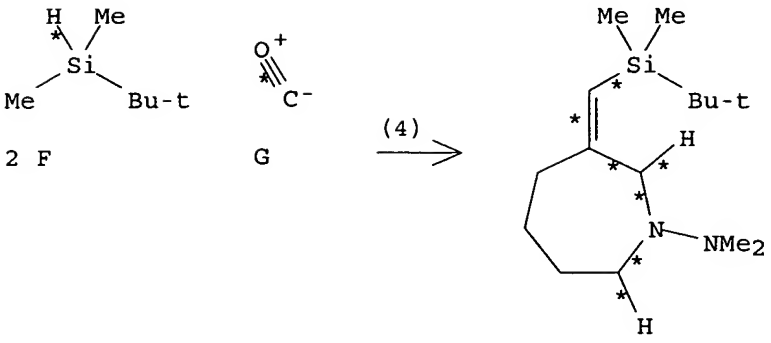
RX(4) OF 16 ...2 M + 2 **F** + G ===> **N** + **O**



M

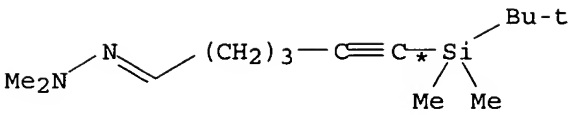


M



2 F G N

YIELD 16%

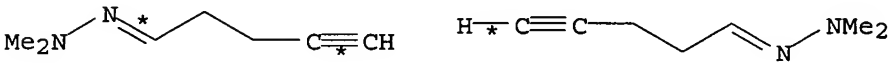


O

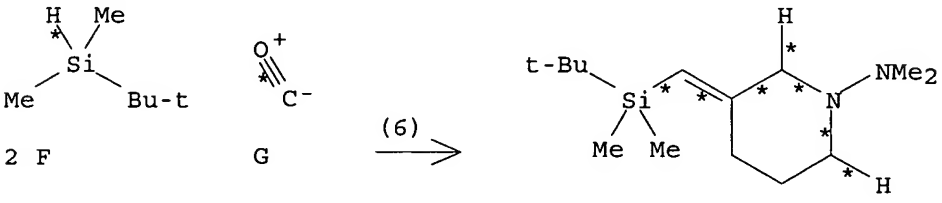
YIELD 42%

RX(4) RCT M 168557-50-4, F **29681-57-0**, G 630-08-0
PRO N **168557-51-5**, O **168557-52-6**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure

RX(6) OF 16 ...2 Q + 2 **F** + G ===> **R** + **S**

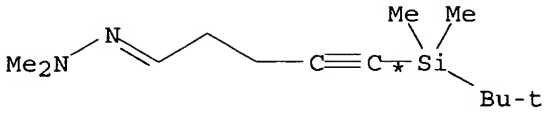


Q Q



2 F G R

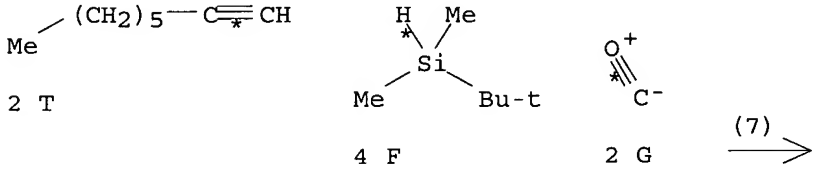
YIELD 24%



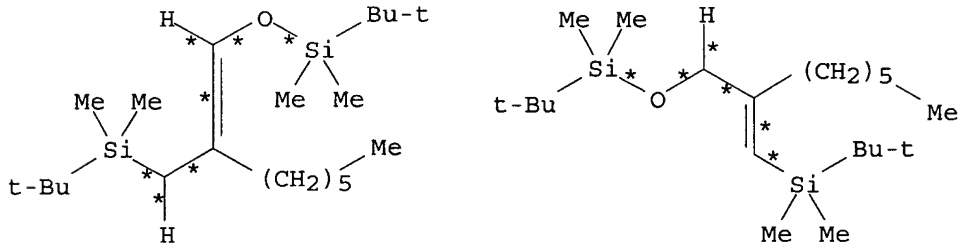
S
YIELD 24%

RX(6) RCT Q 168557-53-7, F **29681-57-0**, G 630-08-0
PRO R **168557-54-8**, S **168557-55-9**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure

RX(7) OF 16 2 T + 4 **F** + 2 G ===> **U** + **V**



2 T 4 F 2 G (7)

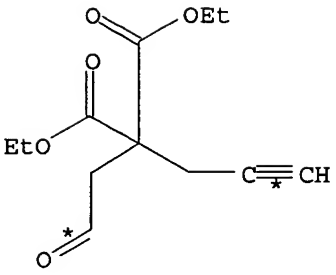


U
YIELD 20%

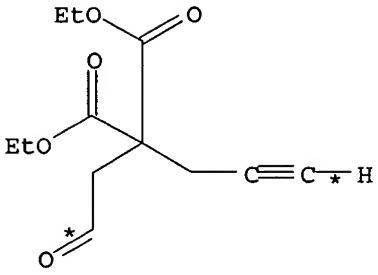
V
YIELD 7%

RX(7) RCT T 629-05-0, F **29681-57-0**, G 630-08-0
PRO U **168557-57-1**, V **168557-56-0**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE high pressure, other product(s) also detected

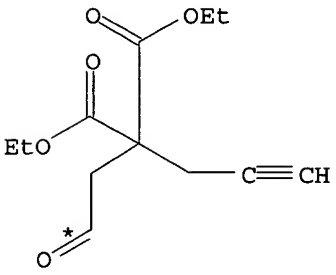
RX(11) OF 16 COMPOSED OF RX(1), RX(2)
RX(11) 3 A + 2 B + 2 C + 2 **F** + G ===> **H** + **I**



A



A



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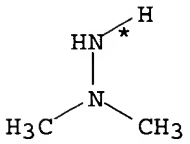
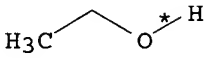
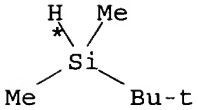


2 B



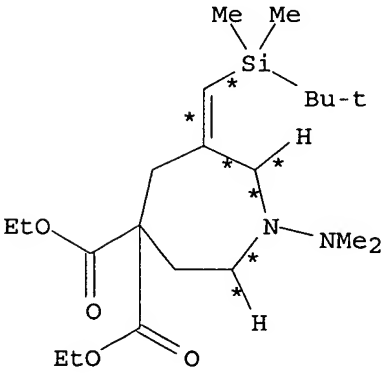
2 C



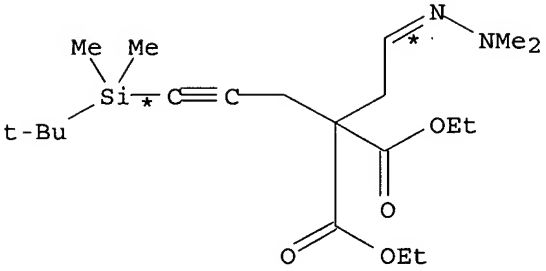
2 F

G

2
STEPS



H
YIELD 53%



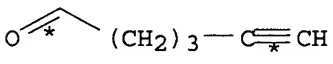
I
YIELD 8%

RX(1) RCT A 137435-59-7, B 57-14-7, C 64-17-5

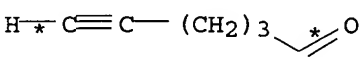
PRO D 168557-46-8, E 168557-58-2
SOL 64-17-5 EtOH

RX(2) RCT D 168557-46-8, F **29681-57-0**, G 630-08-0
PRO H **168557-47-9**, I **168557-48-0**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure, optimization study, optimized on reaction temperature,pressure of CO,catalyst

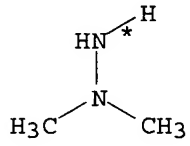
RX(13) OF 16 COMPOSED OF RX(3), RX(4)
RX(13) 2 L + 2 B + 2 **F** + G ===> **N** + **O**



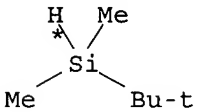
L



L



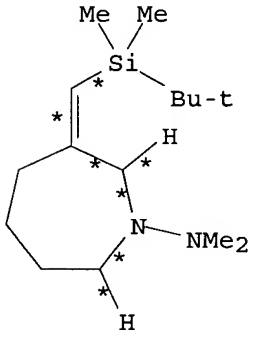
2 B



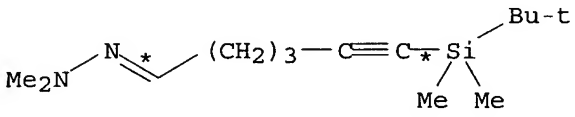
2 F

G

2
STEPS



N
YIELD 16%

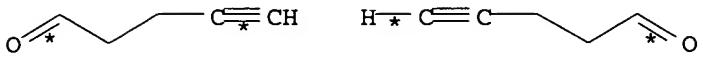


O
YIELD 42%

RX(3) RCT L 29329-03-1, B 57-14-7
PRO M 168557-50-4

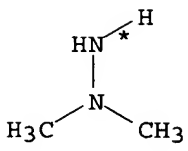
RX(4) RCT M 168557-50-4, F **29681-57-0**, G 630-08-0
PRO N **168557-51-5**, O **168557-52-6**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure

RX(14) OF 16 COMPOSED OF RX(5), RX(6)
RX(14) 2 P + 2 B + 2 **F** + G ===> **R** + **S**

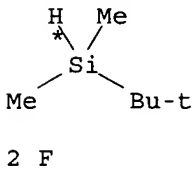


P

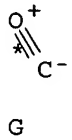
P



2 B

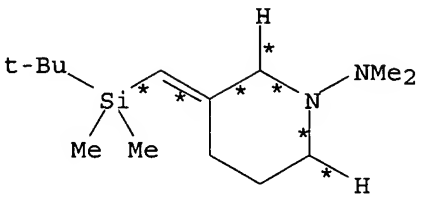


2 F

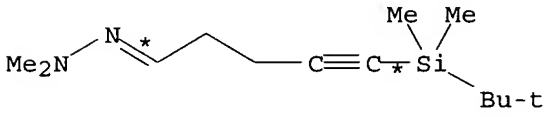


G

2
STEPS



R
YIELD 24%



S
YIELD 24%

RX(5) RCT P 18498-59-4, B 57-14-7
PRO Q 168557-53-7

RX(6) RCT Q 168557-53-7, F **29681-57-0**, G 630-08-0
PRO R **168557-54-8**, S **168557-55-9**
CAT **18827-81-1** Iridium, dodecacarbonyltetra-, tetrahedro
SOL 75-05-8 MeCN
NTE stereoselective, high pressure

L64 ANSWER 23 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:409220 HCAPLUS
DOCUMENT NUMBER: 144:412697
TITLE: Improved process for preparation of organosilanes by hydrosilylation of **alkenes** in the presence of iridium **diene** catalysts and oxidative cocatalysts
INVENTOR(S): Baumann, Frank; Hofmann, Marco
PATENT ASSIGNEE(S): Wacker-Chemie G.m.b.H., Germany
SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006045533	A1	20060504	WO 2005-EP11300	20051020
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004052424	A1	20060504	DE 2004-102004052424	20041028
PRIORITY APPLN. INFO.:			DE 2004-102004052424A	20041028
			DE 2005-102005030581A	20050630

AB An improved process for preparation of alkylsilanes R6R5CHR4CHSiR1R2R3 [R1, R2, R3 = C1-18 alkyl(oxy), preferably R1, R2, R3 = (un)branched C1-6 alkyl, C1-6 alkoxy; R4, R5, R6 = H, organyl, optionally substituted by halo, (alkyl)amino, cyano, CN, NCO], useful as adhesives, crosslinking agents or intermediates (no data), comprises hydrosilylation of **alkenes** R6R5C:CHR4 by silanes HSiR1R2R3, preferably by chlorodimethylsilane, at 1:1.1 to 1:1.25 mol ratio, in the presence of iridium **diene** catalysts, preferably in the presence of di-μ-chlorobis[(1,2,5,6-η)-1,5-**cyclooctadiene**]diiridium and oxidative cocatalysts chosen from inorg. or organometallic oxidants, preferably ferrocenium, [Ru(bipy)3]3+ and [Fe(phen)3]3+, organic oxidants chosen from aldehydes, ketones, diones peroxides, peracids, phosphine oxides, sulfones, tritylium and tropylium salts, taken in 0.5-5 wt% to the reactants, in a **continuous** reactor at 0-200°, preferably at 25-40° at 1-20 atm pressure, preferably as solvent-free process. In an example, a mixture of 0.562 mol of allyl chloride with 70 mg of [(cod)IrCl]2 was reacted with a mixture of 56 g of Me2SiClH and 2 g of acetone as cocatalyst at 90° for 0.5 h, yielding 70% of chloro(3-chloropropyl)dimethylsilane.

CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 45

ST silane alkyl prepn process hydrosilylation **alkene** iridium oxidant catalyst; alkylsilane improved process prepn **alkene** hydrosilylation oxidative cocatalyst; solvent free **continuous** process alkylsilane prepn iridium catalyzed hydrosilylation; ketone dione peroxide cocatalyst hydrosilylation iridium catalyst improved process

IT Silanes
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(alkoxy; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Silanes
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(alkyl; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Ketones, uses
RL: CAT (Catalyst use); USES (Uses)
(diketones; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors
(flow; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Hydrosilylation
Oxidizing agents
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Aldehydes, uses
Ketones, uses
RL: CAT (Catalyst use); USES (Uses)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT **Alkenes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors
(loop; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors
(microreactors; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Peroxides, uses
RL: CAT (Catalyst use); USES (Uses)
(organic; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Carboxylic acids, uses
RL: CAT (Catalyst use); USES (Uses)
(peroxy; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT Reactors
(tubular; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow

reactors and microreactors)

IT 67-64-1, Acetone, uses 100-52-7, Benzaldehyde, uses 108-10-1, Methyl isobutyl ketone 110-05-4, Di-tert-butyl peroxide 123-54-6, Acetylacetone, uses 130-15-4, 1,4-Naphthoquinone 134-81-6, Benzil 504-02-9, 1,3-Cyclohexanedione 637-88-7, 1,4-Cyclohexanedione 765-87-7, 1,2-Cyclohexanedione 7553-56-2, Iodine, uses 7722-64-7, Potassium permanganate 7726-95-6, Bromine, uses 7775-27-1, Sodium peroxodisulfate 7778-50-9, Potassium bichromate 7782-44-7, Oxygen, uses 7782-50-5, Chlorine, uses 7789-00-6, Potassium chromate 10466-65-6, Potassium perrhenate 12125-80-3, Ferrocenium 13479-49-7 13746-66-2, Tripotassium hexacyanoferrate 18955-01-6 31067-25-1, 1,9-Cyclohexadecanedione
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst; improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT **75-78-5P**, Dichlorodimethylsilane **17477-29-1P**, Chlorodimethylpropylsilane
RL: BYP (Byproduct); **PREP (Preparation)**
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

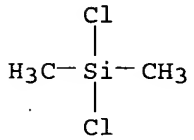
IT **12112-67-3**, Chloro(1,5-**cyclooctadiene**)iridium dimer
RL: **CAT (Catalyst use)**; USES (Uses)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT 107-05-1, Allyl chloride **1066-35-9**, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

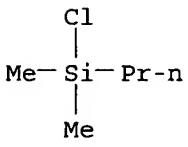
IT **10605-40-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

IT **75-78-5P**, Dichlorodimethylsilane **17477-29-1P**, Chlorodimethylpropylsilane
RL: BYP (Byproduct); **PREP (Preparation)**
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)

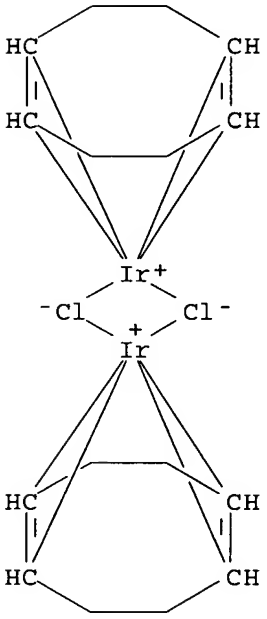
RN 75-78-5 HCAPLUS
CN Silane, dichlorodimethyl- (8CI, 9CI) (CA INDEX NAME)



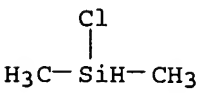
RN 17477-29-1 HCAPLUS
CN Silane, chlorodimethylpropyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



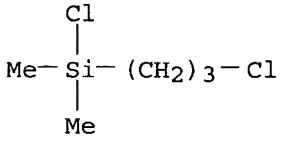
IT **12112-67-3**, Chloro(1,5-**cyclooctadiene**)iridium dimer
RL: **CAT (Catalyst use)**; USES (Uses)
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



IT **1066-35-9**, Chlorodimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **10605-40-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(improved process for preparation of alkylsilanes by solvent-free hydrosilylation of **alkenes** catalyzed by iridium **diene** complexes and oxidative cocatalysts in **continuous** flow reactors and microreactors)
RN 10605-40-0 HCAPLUS
CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



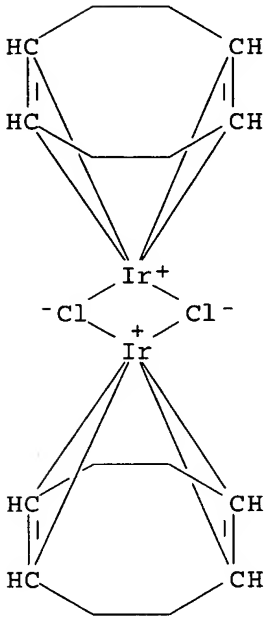
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 24 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:449533 HCAPLUS
DOCUMENT NUMBER: 142:463198
TITLE: Stabilization method of iridium catalyst solution
INVENTOR(S): Tonomura, Yoichi; Kiyomori, Ayumu; Kubota, Toru
PATENT ASSIGNEE(S): Shin-Etsu Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

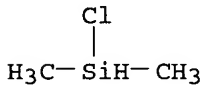
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005131454	A2	20050526	JP 2003-367190	20031028
PRIORITY APPLN. INFO.:			JP 2003-367190	20031028

OTHER SOURCE(S): MARPAT 142:463198
AB The invention refers to a stabilization method of an Ir catalyst solution used in hydrosilylation reactions, wherein a hydroxyl compound R1OH [R1 = C1-20 (un)substituted monovalent hydrocarbon] is added to the solution
IC ICM B01J033-00
ICS B01J031-22; C07F015-00
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 67
IT 64-17-5, Ethanol, uses 104-76-7, 2-Ethyl-1-hexanol 150-76-5, 4-Methoxyphenol **12112-67-3**
RL: **CAT (Catalyst use)**; DEV (Device component use); USES (Uses)
(stabilization method of iridium catalyst solution)
IT 96-05-9, Allyl methacrylate **1066-35-9**, Dimethylchlorosilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(stabilization method of iridium catalyst solution)
IT **24636-31-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(stabilization method of iridium catalyst solution)
IT **12112-67-3**
RL: **CAT (Catalyst use)**; DEV (Device component use); USES (Uses)
(stabilization method of iridium catalyst solution)

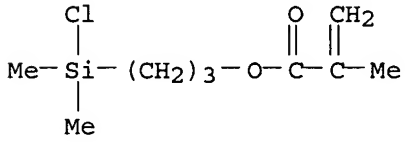
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



IT **1066-35-9**, Dimethylchlorosilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(stabilization method of iridium catalyst solution)
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **24636-31-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(stabilization method of iridium catalyst solution)
RN 24636-31-5 HCAPLUS
CN 2-Propenoic acid, 2-methyl-, 3-(chlorodimethylsilyl)propyl ester (9CI) (CA INDEX NAME)



L64 ANSWER 25 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1335585 HCAPLUS
DOCUMENT NUMBER: 144:51711

TITLE: Improved process for controlled hydrolysis of residues from preparation of an ω-haloalkyl dialkylhalosilanes with subsequent regeneration of platinum-group metal catalyst
INVENTOR(S): Ramdani, Kamel
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: Fr. Demande, 19 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2871802	A1	20051223	FR 2004-6502	20040616
WO 2006003323	A1	20060112	WO 2005-FR1469	20050614

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: FR 2004-6502 A 20040616
OTHER SOURCE(S): MARPAT 144:51711

AB ω-Haloalkyl dialkylhalosilanes of formula XR2R3Si(CH2)sX [1, X = Cl, Br, I, preferably X = Cl; R2, R3 = C1-6 (un)branched alkyl, Ph; S = 2-10; preferably R2 = R3 = Me, s = 3] were prepared by hydrosilylation of **alkenes** CH2:CH(CH2)s-2X (same s, X) catalyzed by platinum-group metal compound, preferably of the type [Ir(R4)X]2 [R4 = unsatd. C4-30 hydrocarbon having 1-8 double or triple bonds; same X]; the improved process, comprises separation of the reaction product 1 by distillation, controlled hydrolysis of the residue containing 40-50% of total halogen and 15-25% of ionizable halogen by addition of 1-5 mol (preferably 1-3 mol) of water per mol of hydrolyzable halogen (Y) at 40-60° with 0.002-0.015 mol H2O min-1 (mol Y)-1, under stirring rate of 200-600 rpm and inert gas bubbling with the debit of 10-50 g h-1. In an example, the controlled hydrolysis of the distillation residue containing 20% of hydrolyzable Cl (2.25 mol) and 1.2 wt% of Ir catalyst at 50° was performed by addition of 120 g of H2O (0.400 g min-1 addition rate) in 1 L reactor with stirring at 400 rpm and bubbling of argon with 14 g h-1 rate; the final content of Cl was 0.13 wt%. The invented method of hydrolysis produces monophasic product, from which the regeneration of Ir catalyst is may be performed without adsorption on solid adsorbent.

IC ICM C07F007-12
CC 29-6 (Organometallic and Organometalloidal Compounds)
IT **12111-11-4 12112-67-3**, Di-μ-chlorobis(1,5-**cyclooctadiene**)diiridium **12245-73-7 60255-04-1 60255-25-6 60255-27-8 656240-93-6 656240-94-7 656240-95-8 656240-96-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(improved process for controlled hydrolysis and hydrogen halide removal

in treatment of platinum-group metal catalyzed hydrosilylation residues)

IT 107-05-1, Allyl chloride **1066-35-9**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

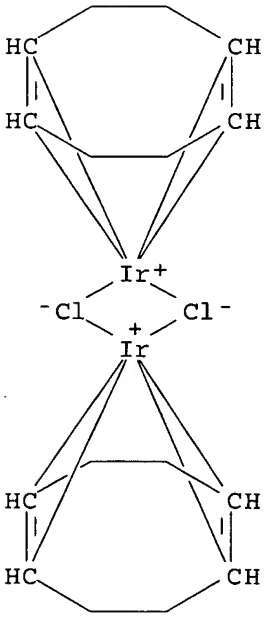
IT **10605-40-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

IT **12111-11-4 12112-67-3**, Di-μ-chlorobis(1,5-**cyclooctadiene**)diiridium **12245-73-7 60255-04-1 60255-25-6 60255-27-8 656240-93-6 656240-94-7 656240-95-8 656240-96-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)

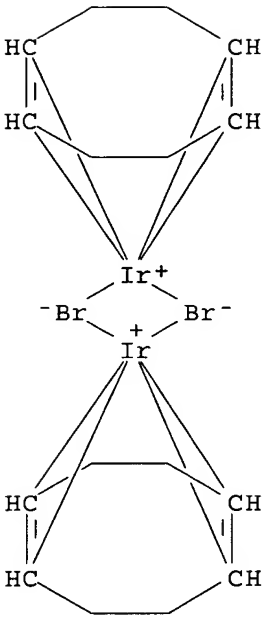
RN 12111-11-4 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

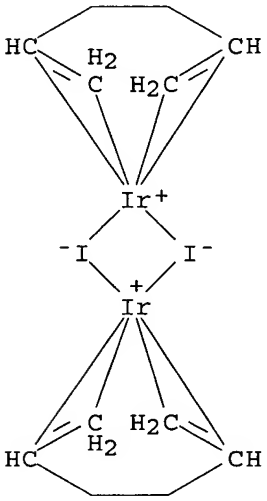
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



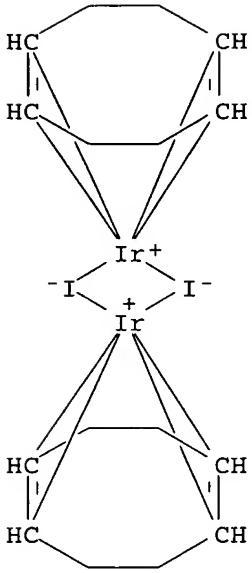
RN 12245-73-7 HCAPLUS
CN Iridium, di-μ-bromobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



RN 60255-04-1 HCAPLUS
CN Iridium, bis[(1,2,5,6-η)-1,5-hexadiene]di-μ-iododi- (9CI) (CA INDEX NAME)

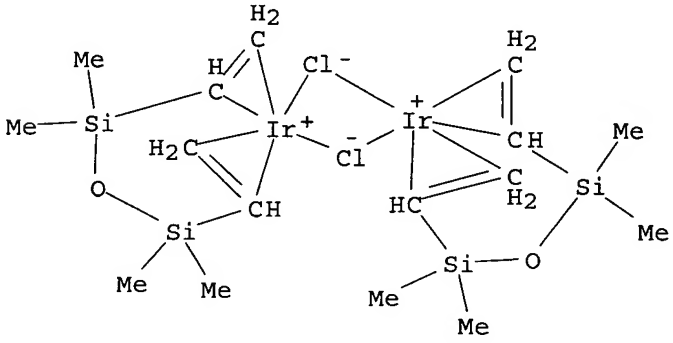


RN 60255-25-6 HCAPLUS
CN Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-iododi- (9CI) (CA INDEX NAME)

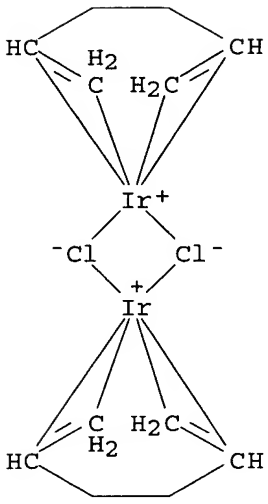


RN 60255-27-8 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-iododi- (9CI) (CA INDEX NAME)

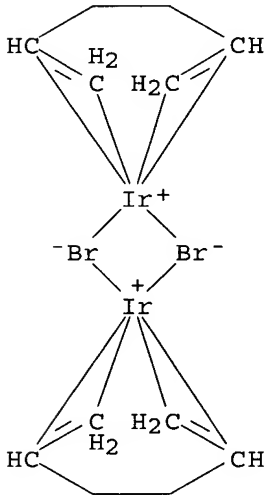
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 656240-93-6 HCAPLUS
CN Iridium, di-μ-chlorobis(η4-1,3-diethenyl-1,1,3,3-tetramethyldisiloxane)di- (9CI) (CA INDEX NAME)



RN 656240-94-7 HCAPLUS
CN Iridium(2+), di-μ-chlorobis[(1,2,5,6-η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)

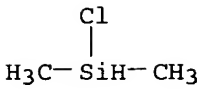


RN 656240-95-8 HCAPLUS
CN Iridium, di-μ-bromobis[(1,2,5,6-η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)

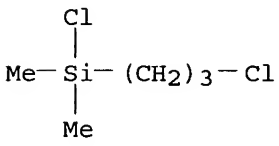


RN 656240-96-9 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-bromodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **1066-35-9**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **10605-40-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(improved process for controlled hydrolysis and hydrogen halide removal in treatment of platinum-group metal catalyzed hydrosilylation residues)
RN 10605-40-0 HCAPLUS
CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 26 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1089559 HCAPLUS
DOCUMENT NUMBER: 143:347293
TITLE: Preparation of (chloropropyl)trialkoxysilane from trialkoxysilane
INVENTOR(S): Xu, Qimin; Xu, Chenggong; Zhang, Zhenglin; Yan, Zeliang; Yang, Yaping
PATENT ASSIGNEE(S): Jurong Xingchun Chemical Co., Ltd., Peop. Rep. China; Southeast University
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 5 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1563015	A	20050112	CN 2004-10014296	20040312

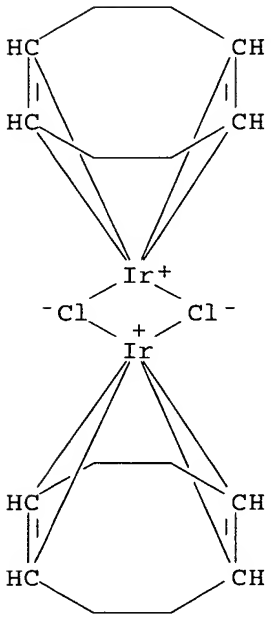
PRIORITY APPLN. INFO.: CN 2004-10014296 20040312
OTHER SOURCE(S): CASREACT 143:347293

AB The invention discloses a process for preparing chloropropyltrialkoxysilane directly from trialkoxysilane, which comprises adding weighted trialkoxysilane into silane solvent (0.2-2 times the mass of trialkoxysilane) in the presence of transition metal compound or its alc. solution as catalyst (1-1,000 ppm the mass of trialkoxysilane calculated on the basis of metal ion) and protective nitrogen, reacting for 1-10 h at room temperature, adding chloropropene 1/3-10/3 the mole number of trialkoxysilane, heating to 25-150°C to allow the reaction to proceed for 2-4 h, adding dropwise chloropropene 1/5-1/20 the mole number of trialkoxysilane, maintaining the temperature for 1-3 h, and separating to obtain the final product.

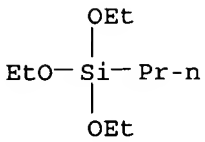
In the invention, the transition metal compound is used as catalyst to achieve homogeneous catalysis.

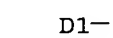
IC ICM C07F007-18

CC 29-6 (Organometallic and Organometalloidal Compounds)
IT 10025-83-9, Iridium chloride 10049-08-8, Ruthenium trichloride **12112-67-3**, **Cyclooctadiene** iridium chloride dimer 14996-61-3, Iridium trichloride hydrate 15243-33-1, Triruthenium dodecacarbonyl 16941-92-7, Chloroiridic acid 20765-98-4, Rhodium chloride hydrate
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound)
IT **29656-55-1P**, Chloropropyltriethoxysilane
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound)
IT 107-05-1, Allyl chloride **998-30-1**, Triethoxysilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound)
IT **12112-67-3**, **Cyclooctadiene** iridium chloride dimer
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound)
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)

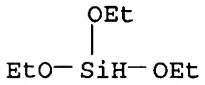


IT **29656-55-1P**, Chloropropyltriethoxysilane
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound)
RN 29656-55-1 HCAPLUS
CN Silane, (chloropropyl)triethoxy- (9CI) (CA INDEX NAME)





IT **998-30-1**, Triethoxysilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of chloropropyltralkoxysilane by hydrosilylation of allyl chloride with trialkoxysilane in presence of transition metal compound).
RN 998-30-1 HCAPLUS
CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



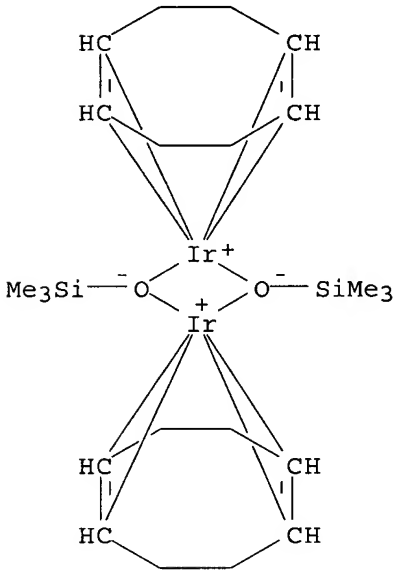
L64 ANSWER 27 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:104757 HCAPLUS
DOCUMENT NUMBER: 143:26955
TITLE: Synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization
AUTHOR(S): Pawluc, Piotr; Marciniec, Bogdan; Kownacki, Ireneusz; Maciejewski, Hieronim
CORPORATE SOURCE: Department of Organometallic Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Poznan, 60-780, Pol.
SOURCE: Applied Organometallic Chemistry (2005), 19(1), 49-54
CODEN: AOCHEX; ISSN: 0268-2605
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB New phenylene-silylene-ethylene polymers were successfully synthesized using platinum-divinylsiloxane or rhodium and iridium siloxane complex-catalyzed polyhydrosilylation of divinylsubstituted carbosilanes with dihydrocarbosilanes or intermol. hydrosilylation of new hydrovinylcarbosilane. Polycarbosilanes have been obtained with high mol. wts. They seem to be potential parent substances for future applications as preceramic and membrane materials.
CC 35-5 (Chemistry of Synthetic High Polymers)
IT 11057-89-9 158240-74-5 **448963-53-9** 463967-39-7 681485-46-1
RL: **CAT (Catalyst use)**; USES (Uses)
(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)
IT 106-37-6 **1066-35-9** 1637-65-6 1826-67-1 13528-93-3
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)
IT **1719-58-0P 20152-11-8P 851479-30-6P**
852699-35-5P 852699-36-6P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

IT **851479-31-7P 851479-32-8P 851479-33-9P**
852699-37-7P 852699-38-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

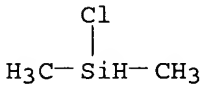
IT **448963-53-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

RN 448963-53-9 HCAPLUS
CN Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]bis[μ-(trimethylsilanolato)]di- (9CI) (CA INDEX NAME)



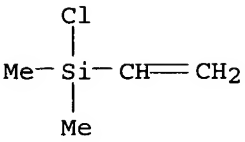
IT **1066-35-9**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

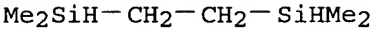


IT **1719-58-0P 20152-11-8P 851479-30-6P**
852699-35-5P 852699-36-6P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

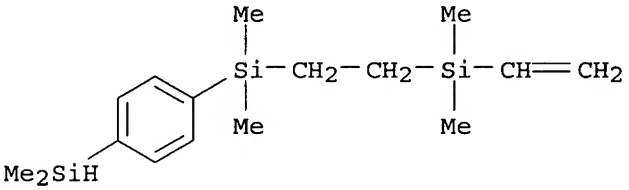
RN 1719-58-0 HCAPLUS
CN Silane, chloroethenyldimethyl- (9CI) (CA INDEX NAME)



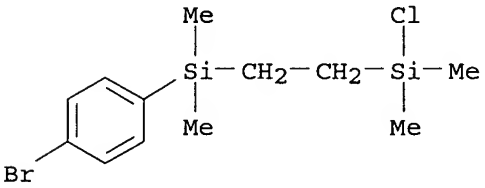
RN 20152-11-8 HCAPLUS
CN Silane, 1,2-ethanediylbis[dimethyl- (9CI) (CA INDEX NAME)



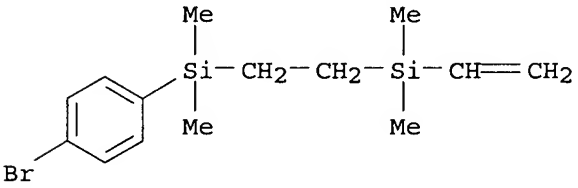
RN 851479-30-6 HCAPLUS
CN Silane, [4-(dimethylsilyl)phenyl][2-(ethenyldimethylsilyl)ethyl]dimethyl- (9CI) (CA INDEX NAME)



RN 852699-35-5 HCAPLUS
CN Silane, (4-bromophenyl)[2-(chlorodimethylsilyl)ethyl]dimethyl- (9CI) (CA INDEX NAME)



RN 852699-36-6 HCAPLUS
CN Silane, [2-[(4-bromophenyl)dimethylsilyl]ethyl]ethenyldimethyl- (9CI) (CA INDEX NAME)



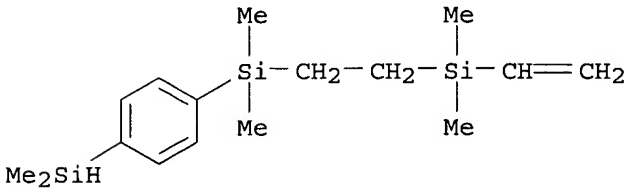
IT **851479-31-7P 851479-32-8P 851479-33-9P**
852699-37-7P 852699-38-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**

(synthesis of phenylene-silylene-ethylene polymers via transition metal complex catalyzed hydrosilylation polymerization)

RN 851479-31-7 HCAPLUS
CN Silane, [4-(dimethylsilyl)phenyl][2-(ethenyldimethylsilyl)ethyl]dimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

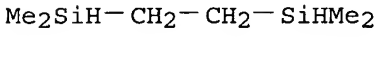
CRN 851479-30-6
CMF C16 H30 Si3



RN 851479-32-8 HCAPLUS
CN Silane, 1,2-ethanediylbis[dimethyl-, polymer with 1,4-phenylenebis[ethenyldimethylsilane] (9CI) (CA INDEX NAME)

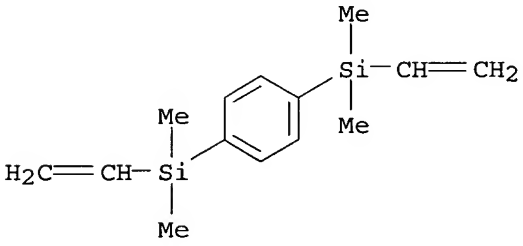
CM 1

CRN 20152-11-8
CMF C6 H18 Si2



CM 2

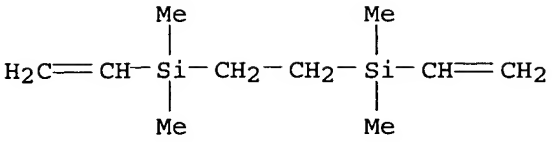
CRN 4519-17-9
CMF C14 H22 Si2



RN 851479-33-9 HCAPLUS
CN Silane, 1,2-ethanediylbis[ethenyldimethyl-, polymer with 1,4-phenylenebis[dimethylsilane] (9CI) (CA INDEX NAME)

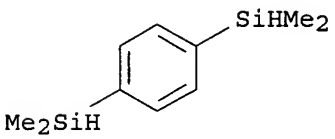
CM 1

CRN 84677-98-5
CMF C10 H22 Si2

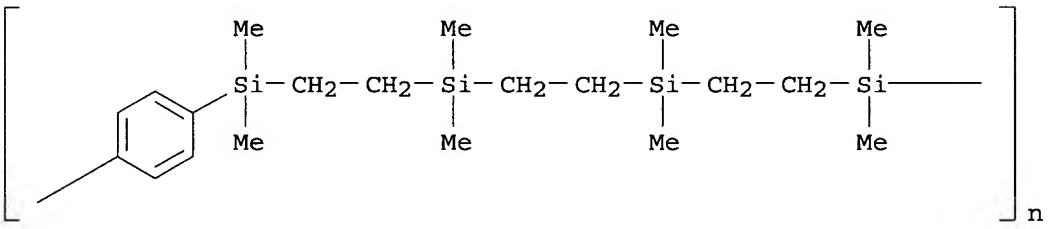


CM 2

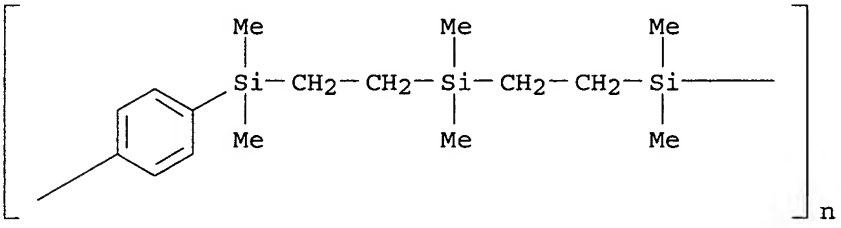
CRN 2488-01-9
CMF C10 H18 Si2



RN 852699-37-7 HCAPLUS
CN Poly[(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,4-phenylene] (9CI) (CA INDEX NAME)



RN 852699-38-8 HCAPLUS
CN Poly[(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,2-ethanediyl(dimethylsilylene)-1,4-phenylene] (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 28 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:120515 HCAPLUS
DOCUMENT NUMBER: 140:164015

TITLE: Process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of iridium catalyst and subsequent catalyst recovery
INVENTOR(S): Guennouni, Nathalie; Ramdani, Kamel
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: Fr. Demande, 19 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2843391	A1	20040213	FR 2002-10146	20020809
FR 2843391	B1	20040910		
FR 2843392	A1	20040213	FR 2003-284	20030113
FR 2843392	B1	20040910		
WO 2004016628	A1	20040226	WO 2003-FR2301	20030721
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003269042	A1	20040303	AU 2003-269042	20030721
EP 1554291	A1	20050720	EP 2003-750829	20030721
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.:

FR 2002-10146	A	20020809
FR 2003-284	A	20030113
WO 2003-FR2301	W	20030721

OTHER SOURCE(S): MARPAT 140:164015

AB Haloalkyl(dialkyl)chlorosilanes XSi(RR1)(CH2)sX [X = Cl, Br, iodo; R, R1 = (un)branched C1-6 alkyl, Ph; s = 2-10] are prepared by hydrosilylation of alkenyl halides CH2:CH(CH2)s-2X (same X, s) with silanes XSi(RR1)H (same X, R, R1) in the presence of a platinum-group metal catalyst, preferably an iridium complex [Ir(R2)X]2 (same X, R2 = unsatd. C4-30 hydrocarbyl containing at least 1 C:C double bond and or C.tplbond.C triple bond), such that the reaction medium is distilled to sep. the product from distillation bottoms comprising byproducts and the platinum-group metal or its derivs., whereupon the bottoms are contacted with a solid substance effective in adsorbing the platinum-group metal, and subsequent separation of the adsorbent from the platinum-group metal to recover the metal. Examples are given for recovery of catalysts based on Ir by using carbon black 2S as adsorbent following synthesis of 3-chloropropyl(dimethyl)chlorosilane.

IC ICM C07F007-14
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 45
IT 7439-88-5P, Iridium, preparation 7440-04-2P, Osmium, preparation 7440-05-3P, Palladium, preparation 7440-06-4P, Platinum, preparation 7440-18-8P, Ruthenium, preparation **12111-11-4P** **12112-67-3P** **12245-73-7P** **60255-04-1P** **60255-25-6P** **60255-27-8P** **656240-93-6P**

656240-94-7P 656240-95-8P 656240-96-9P
RL: **CAT (Catalyst use)**; PUR (Purification or recovery); PREP (Preparation); USES (Uses)
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

IT **10605-40-0P**, Chloro(3-chloropropyl)dimethylsilane
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

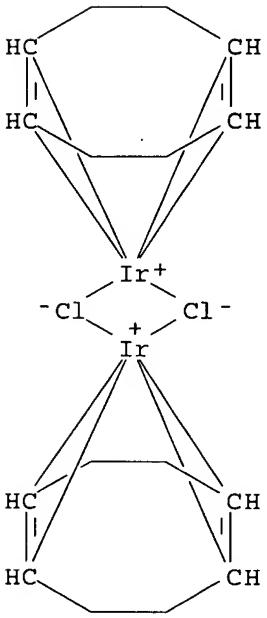
IT 107-05-1, Allyl chloride **1066-35-9**, Chloro(dimethyl)silane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

IT **12111-11-4P 12112-67-3P 12245-73-7P**
60255-04-1P 60255-25-6P 60255-27-8P
656240-93-6P 656240-94-7P 656240-95-8P
656240-96-9P
RL: **CAT (Catalyst use)**; PUR (Purification or recovery); PREP (Preparation); USES (Uses)
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)

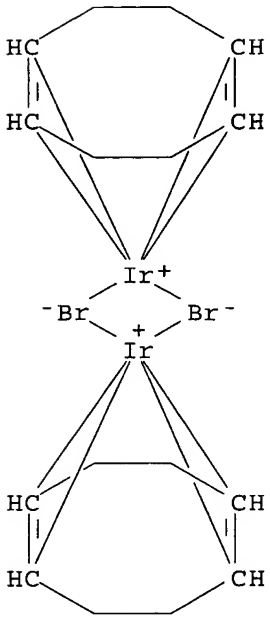
RN 12111-11-4 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

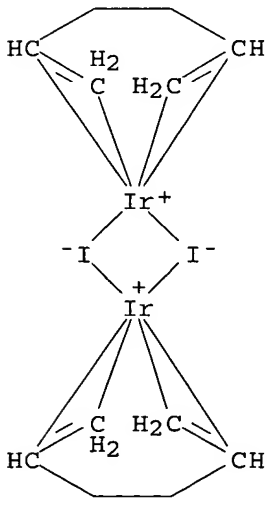
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



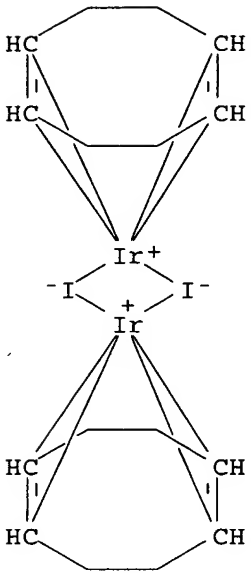
RN 12245-73-7 HCAPLUS
CN Iridium, di-μ-bromobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



RN 60255-04-1 HCAPLUS
CN Iridium, bis[(1,2,5,6-η)-1,5-hexadiene]di-μ-iododi- (9CI) (CA INDEX NAME)

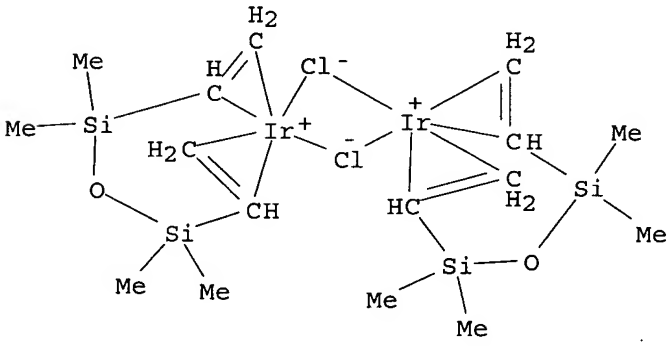


RN 60255-25-6 HCAPLUS
CN Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-iododi- (9CI) (CA INDEX NAME)

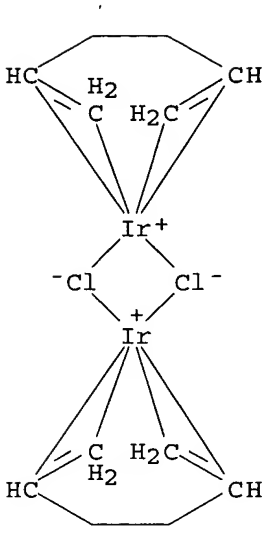


RN 60255-27-8 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-iododi- (9CI) (CA INDEX NAME)

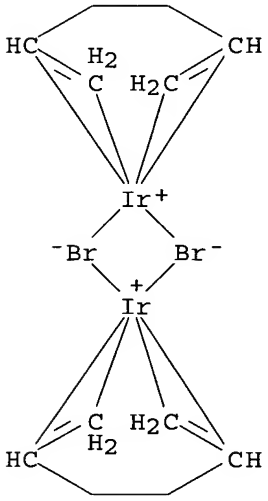
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 656240-93-6 HCAPLUS
CN Iridium, di-μ-chlorobis(η4-1,3-diethenyl-1,1,3,3-tetramethyldisiloxane)di- (9CI) (CA INDEX NAME)



RN 656240-94-7 HCAPLUS
CN Iridium(2+), di-μ-chlorobis[(1,2,5,6-η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)

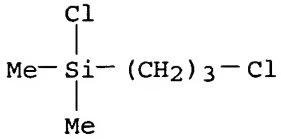


RN 656240-95-8 HCAPLUS
CN Iridium, di-μ-bromobis[(1,2,5,6-η)-1,5-hexadiene]di- (9CI) (CA INDEX NAME)

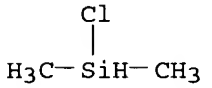


RN 656240-96-9 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-bromodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **10605-40-0P**, Chloro(3-chloropropyl)dimethylsilane
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)
RN 10605-40-0 HCAPLUS
CN Silane, chloro(3-chloropropyl)dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **1066-35-9**, Chloro(dimethyl)silane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(process for preparation of haloalkyl(dialkyl)chlorosilanes by hydrosilylation of alkenyl halides in presence of platinum-group catalyst and subsequent catalyst recovery)
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 29 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:769875 HCAPLUS
DOCUMENT NUMBER: 141:424227
TITLE: Ru3(CO)12-Catalyzed Silylation of Benzylic C-H Bonds in Arylpyridines and Arylpyrazoles with Hydrosilanes via C-H Bond Cleavage
AUTHOR(S): Kakiuchi, Fumitoshi; Tsuchiya, Kazuyuki; Matsumoto, Mitsutaka; Mizushima, Eiichiro; Chatani, Naoto
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Osaka University, Osaka, 565-0871, Japan
SOURCE: Journal of the American Chemical Society (2004), 126(40), 12792-12793
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:424227
AB Ruthenium-catalyzed silylation of sp3 C-H bonds at a benzylic position with hydrosilanes gave benzylsilanes. For this silylation reaction, Ru3(CO)12 complex showed high catalytic activity. This silylation proceeded at the Me C-H bond selectively. For this silylation reaction, pyridyl and pyrazolyl groups, and the imino group in hydrazones, can function as a directing group. Several hydrosilanes involving triethyl-, dimethylphenyl-, tert-butyldimethyl-, and triphenylsilanes can be used as a silylating reagent. Coordination of an sp2 nitrogen atom to the ruthenium complex is important for achieving this silylation reaction. Thus, Ru3(CO)12/norbornene catalyzed silylation of 2-(2,6-dimethylphenyl)pyridine with Et3SiH in PhMe at reflux gave 30% 2-(2-methyl-6-triethylsilanylmethylphenyl)pyridine along with 55% 2-(2,6-bis-triethylsilanylmethylphenyl)pyridine.
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21
IT 498-66-8, Norbornene **12148-71-9** 13815-94-6, Ruthenium trichloride trihydrate 15243-33-1, Dodecacarbonyltriruthenium

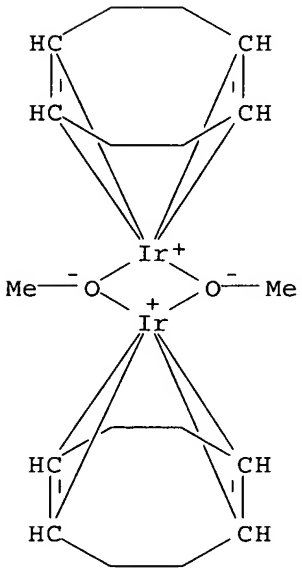
19584-30-6, Tetrarhodium dodecacarbonyl 25360-32-1 52462-29-0
73468-85-6 91739-95-6 91947-90-9
RL: **CAT (Catalyst use)**; USES (Uses)
(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

IT 611-32-5 **617-86-7**, Triethylsilane 766-77-8,
Dimethyl(phenyl)silane 789-25-3, Triphenylsilane 1762-32-9
10273-89-9 10273-91-3 10273-93-5 **29681-57-0**,
tert-Butyldimethylsilane 38581-14-5 706788-75-2 793681-25-1
793681-26-2 793681-27-3 793681-28-4 793681-29-5
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

IT **793681-20-6P 793681-21-7P 793681-22-8P**
793681-23-9P 793681-24-0P 793681-30-8P
793681-31-9P 793681-32-0P 793681-33-1P
793681-34-2P 793681-35-3P 793681-36-4P
793681-37-5P 793681-38-6P 793681-39-7P
793681-40-0P 793681-41-1P 793681-42-2P
793681-43-3P 793681-44-4P 793681-45-5P
793681-46-6P 793681-47-7P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

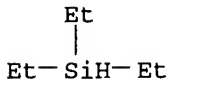
IT **12148-71-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)

RN 12148-71-9 HCAPLUS
CN Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi- (9CI) (CA INDEX NAME)

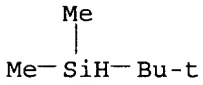


IT **617-86-7**, Triethylsilane **29681-57-0**,

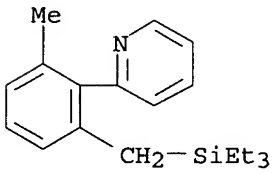
tert-Butyldimethylsilane
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)
RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



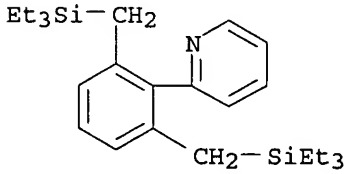
RN 29681-57-0 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



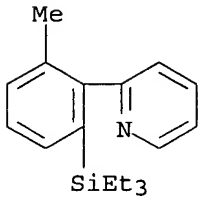
IT **793681-20-6P 793681-21-7P 793681-22-8P**
793681-23-9P 793681-24-0P 793681-30-8P
793681-31-9P 793681-32-0P 793681-34-2P
793681-35-3P 793681-36-4P 793681-37-5P
793681-38-6P 793681-39-7P 793681-40-0P
793681-41-1P 793681-42-2P 793681-43-3P
793681-44-4P 793681-45-5P 793681-46-6P
793681-47-7P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(ruthenium carbonyl catalyzed silylation of benzylic carbon-hydrogen bonds in arylpyridines and arylpyrazoles with hydrosilanes via carbon-hydrogen bond cleavage)
RN 793681-20-6 HCAPLUS
CN Pyridine, 2-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



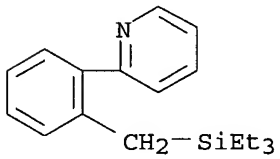
RN 793681-21-7 HCAPLUS
CN Pyridine, 2-[2,6-bis[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



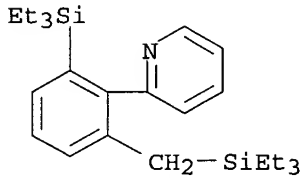
RN 793681-22-8 HCAPLUS
CN Pyridine, 2-[2-methyl-6-(triethylsilyl)phenyl]- (9CI) (CA INDEX NAME)



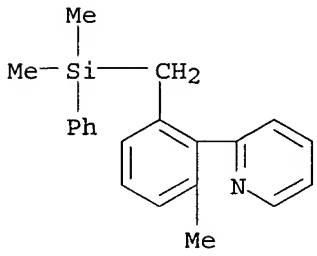
RN 793681-23-9 HCAPLUS
CN Pyridine, 2-[2-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



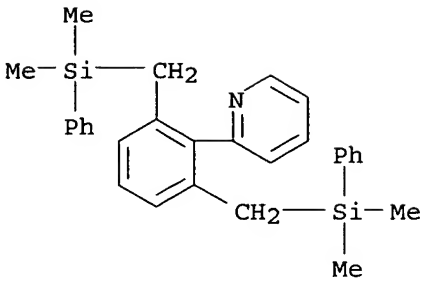
RN 793681-24-0 HCAPLUS
CN Pyridine, 2-[2-(triethylsilyl)-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



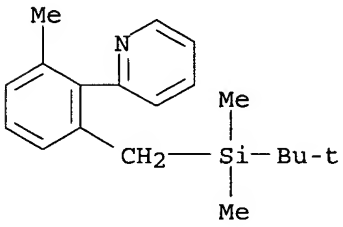
RN 793681-30-8 HCAPLUS
CN Pyridine, 2-[2-[(dimethylphenylsilyl)methyl]-6-methylphenyl]- (9CI) (CA INDEX NAME)



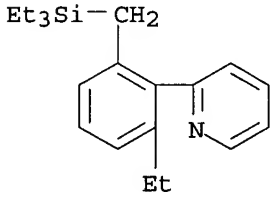
RN 793681-31-9 HCAPLUS
CN Pyridine, 2-[2,6-bis[(dimethylphenylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



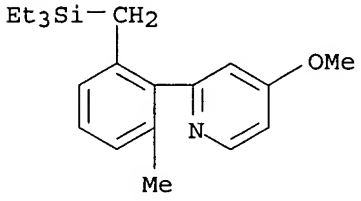
RN 793681-32-0 HCAPLUS
CN Pyridine, 2-[2-[[(1,1-dimethylethyl)dimethylsilyl]methyl]-6-methylphenyl]- (9CI) (CA INDEX NAME)



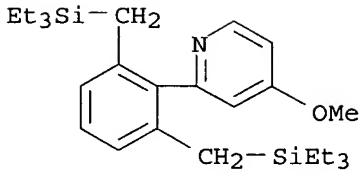
RN 793681-34-2 HCAPLUS
CN Pyridine, 2-[2-ethyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



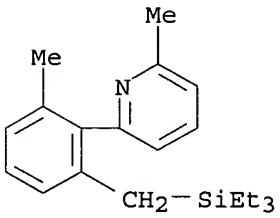
RN 793681-35-3 HCAPLUS
CN Pyridine, 4-methoxy-2-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



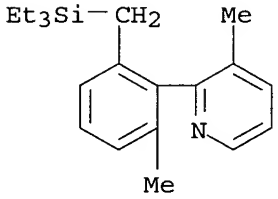
RN 793681-36-4 HCAPLUS
CN Pyridine, 2-[2,6-bis[(triethylsilyl)methyl]phenyl]-4-methoxy- (9CI) (CA INDEX NAME)



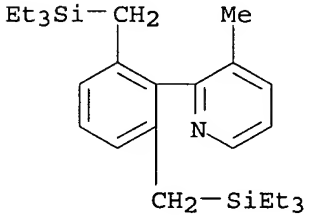
RN 793681-37-5 HCAPLUS
CN Pyridine, 2-methyl-6-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



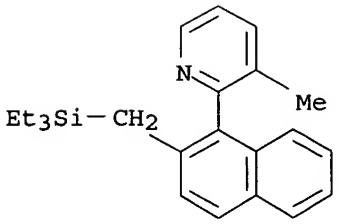
RN 793681-38-6 HCAPLUS
CN Pyridine, 3-methyl-2-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



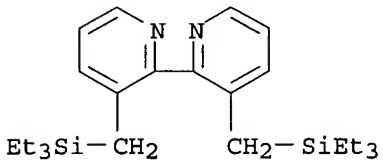
RN 793681-39-7 HCAPLUS
CN Pyridine, 2-[2,6-bis[(triethylsilyl)methyl]phenyl]-3-methyl- (9CI) (CA INDEX NAME)



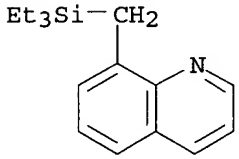
RN 793681-40-0 HCAPLUS
CN Pyridine, 3-methyl-2-[2-[(triethylsilyl)methyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)



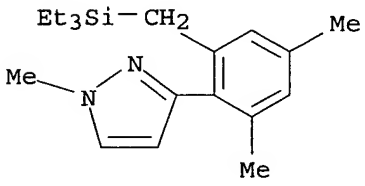
RN 793681-41-1 HCAPLUS
CN 2,2'-Bipyridine, 3,3'-bis[(triethylsilyl)methyl]- (9CI) (CA INDEX NAME)



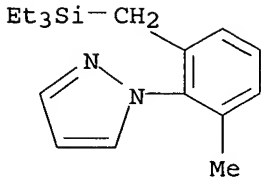
RN 793681-42-2 HCAPLUS
CN Quinoline, 8-[(triethylsilyl)methyl]- (9CI) (CA INDEX NAME)



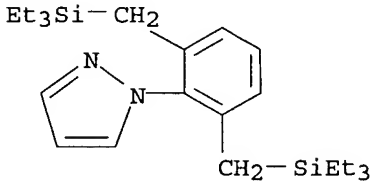
RN 793681-43-3 HCAPLUS
CN 1H-Pyrazole, 3-[2,4-dimethyl-6-[(triethylsilyl)methyl]phenyl]-1-methyl- (9CI) (CA INDEX NAME)



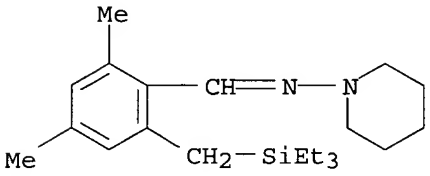
RN 793681-44-4 HCAPLUS
CN 1H-Pyrazole, 1-[2-methyl-6-[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



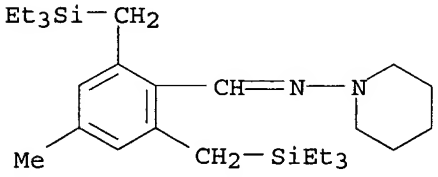
RN 793681-45-5 HCAPLUS
CN 1H-Pyrazole, 1-[2,6-bis[(triethylsilyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 793681-46-6 HCAPLUS
CN 1-Piperidinamine, N-[[2,4-dimethyl-6-[(triethylsilyl)methyl]phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 793681-47-7 HCAPLUS
CN 1-Piperidinamine, N-[[4-methyl-2,6-bis[(triethylsilyl)methyl]phenyl]methylene]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 30 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:16299 HCAPLUS
DOCUMENT NUMBER: 138:136796
TITLE: Selective, Catalytic Carbon-Carbon Bond Activation and Functionalization Promoted by Late Transition Metal Catalysts
AUTHOR(S): Bart, Suzanne C.; Chirik, Paul J.

CORPORATE SOURCE: Department of Chemistry and Chemical Biology Baker Laboratory, Cornell University, Ithaca, NY, 14853, USA
SOURCE: Journal of the American Chemical Society (2003), 125(4), 886-887
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:136796

AB The selective catalytic activation and functionalization of carbon-carbon bonds in a series of substituted cyclopropane substrates has been developed using com. available transition metal catalysts. Catalytic hydrogenation and olefination procedures, tolerant of a range of functional groups, have been discovered. Introduction of a chelate-assisting substituent such as [PPh2] is effective in altering the kinetic selectivity and lowering the activation barrier for the catalytic processes.

CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 67

IT 12080-32-9, Dichloro(1,5-**cyclooctadiene**)platinum 12092-47-6, Dichlorobis(1,5-**cyclooctadiene**)rhodium(I) **12112-67-3**, Dichlorobis(**cyclooctadiene**)diiridium **12246-51-4**, Dichlorotetrakis(cyclooctene)diiridium 13938-94-8, Chlorocarbonylbis(triphenylphosphine)rhodium 14221-01-3, Tetrakis(triphenylphosphine)palladium 14694-95-2, Rhodium tris(triphenylphosphine) chloride
RL: **CAT (Catalyst use)**; USES (Uses)
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)

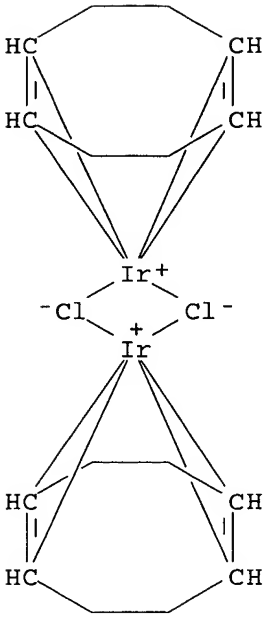
IT 64-67-5, Diethylsulfate 75-36-5, Acetyl chloride 75-77-4, Trimethylsilyl chloride, reactions **617-86-7**, Triethylsilane 930-57-4 1079-66-9, Chlorodiphenylphosphine 2516-33-8, Cyclopropanemethanol 25267-27-0, Iodobutane 473734-58-6
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)

IT 36982-54-4P 70097-81-3P **85696-54-4P** 494769-09-4P 494769-10-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)

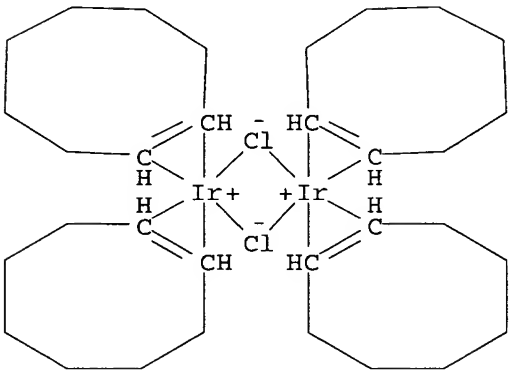
IT 78-83-1P, preparation 110-19-0P 591-76-4P 627-02-1P 820-71-3P 6094-02-6P 17616-98-7P **18269-50-6P** 24309-28-2P **25195-85-1P** 494769-11-8P **494769-12-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)

IT **12112-67-3**, Dichlorobis(**cyclooctadiene**)diiridium **12246-51-4**, Dichlorotetrakis(cyclooctene)diiridium
RL: **CAT (Catalyst use)**; USES (Uses)
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)

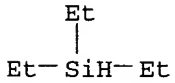
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



RN 12246-51-4 HCAPLUS
CN Iridium, di-μ-chlorotetrakis[(1,2-η)-cyclooctene]di- (9CI) (CA INDEX NAME)



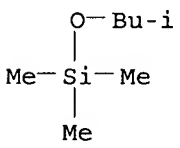
IT **617-86-7**, Triethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)
RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



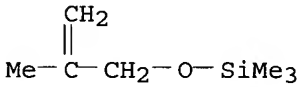
IT **85696-54-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**

(Preparation); RACT (Reactant or reagent)
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)
RN 85696-54-4 HCAPLUS
CN Silane, (cyclopropylmethoxy)trimethyl- (9CI) (CA INDEX NAME)

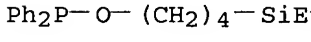
IT **18269-50-6P 25195-85-1P 494769-12-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(selective catalytic carbon-carbon bond activation and functionalization promoted by transition metal catalysts)
RN 18269-50-6 HCAPLUS
CN Silane, trimethyl(2-methylpropoxy)- (9CI) (CA INDEX NAME)



RN 25195-85-1 HCAPLUS
CN Silane, trimethyl[(2-methyl-2-propenyl)oxy]- (9CI) (CA INDEX NAME)



RN 494769-12-9 HCAPLUS
CN Phosphinous acid, diphenyl-, 4-(triethylsilyl)butyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 31 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:71112 HCAPLUS
DOCUMENT NUMBER: 137:47249
TITLE: The effect of oxygen on the regioselectivity in the rhodium catalysed hydrosilylation of 1,3-**dienes**
AUTHOR(S): Gustafsson, Magnus; Frejd, Torbjoern
CORPORATE SOURCE: Organic Chemistry, Centre for Chemistry and Chemical Engineering, Lund University, Lund, S-221 00, Swed.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2002), (1), 102-107
CODEN: JCSPCE; ISSN: 1472-7781
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:47249

AB The regioselectivity of the hydrosilylation of substituted 1,3-**dienes** catalyzed by several Rh complexes in the presence and absence of O2 was studied. In addition to the already known accelerating effect, the presence of O2 strongly affected the product distribution. For 2-substituted 1,3-**dienes** in the presence of O2 the regioselectivity was in the range of 1:6 to 1:10 in favor of the head-product, while the absence of O2 changed the ratios to 1:1 to 3:1 in favor of the tail-product. When HSiPh3 was used in the presence of O2 a single isomer was isolated in 87% yield, while in the absence of O2 a mixture of products was produced. Control expts. indicated that a heterogeneous/colloidal catalytic system may be responsible for the preferred head-product formation.

CC 29-6 (Organometallic and Organometalloidal Compounds)

ST oxygen effect regioselectivity rhodium catalyzed hydrosilylation unsym **diene**

IT **Alkadienes**
RL: RCT (Reactant); RACT (Reactant or reagent)
(1,3-; effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **dienes**)

IT Hydrosilylation
Hydrosilylation catalysts
Regiochemistry
(effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **dienes**)

IT **12112-67-3**, Dichlorobis(1,5-**cyclooctadiene**)diiridium
RL: **CAT (Catalyst use)**; USES (Uses)
(effect of oxygen on regioselectivity in catalyzed hydrosilylation of unsym. **diene**)

IT 13569-65-8, Rhodium trichloride trihydrate 13938-94-8, Carbonyl(chloro)bis(triphenylphosphine)rhodium 14284-92-5, Rhodium tris(acetylacetonate) 14694-95-2, Chlorotris(triphenylphosphine)rhodium 17185-29-4, Carbonylhydrotris(triphenylphosphine)rhodium 18284-36-1, Hydrotetrakis(triphenylphosphine)rhodium 26500-10-7, Chloro(thiocarbonyl)bis(triphenylphosphine)rhodium
RL: CAT (Catalyst use); USES (Uses)
(effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)

IT 78-79-5, Isoprene, reactions 123-35-3, 7-Methyl-3-(methylene)-1,6-**octadiene 617-86-7**, Triethylsilane 766-77-8, Dimethyl(phenyl)silane 789-25-3, Triphenylsilane 926-54-5, (E)-2-Methyl-1,3-**pentadiene** 930-68-7, 2-Cyclohexen-1-one **998-30-1**, Triethoxysilane 2004-70-8, (E)-1,3-**Pentadiene** **2487-90-3**, Trimethoxysilane 29414-55-9, 2,2-Dimethyl-3-(3-(methylene)-4-pentenyl)oxirane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)

IT **18032-09-2P**, 1-Triethylsilyl-3-methylbut-2-ene **35754-76-8P**, 1-Triethoxysilyl-3-methylbut-2-ene **50598-99-7P** **63942-83-6P**, (Z)-1-Triethoxysilyl-2-methylbut-2-ene **63972-14-5P**, 1-[Dimethyl(phenyl)silyl]-3-methylbut-2-ene **68260-36-6P**, (E)-3,7-Dimethyl-1-[dimethyl(phenyl)silyl]octa-2,6-**diene 72142-16-6P**, 1-Trimethoxysilyl-3-methylbut-2-ene **108311-91-7P**, (Z)-1-Triethylsilyl-2-methylbut-2-ene **108311-92-8P**, (Z)-1-Trimethoxysilyl-2-methylbut-2-ene **167314-58-1P**, (Z)-1-[Dimethyl(phenyl)silyl]-2-methylpent-2-ene **438045-62-6P**, (2Z)-1-Cyclohexyl-7-methyl-3-

[dimethyl(phenyl)silylmethyl]octa-2,6-**diene** 438045-63-7P, 3-Methyl-1-triphenylsilylbut-2-ene 438045-64-8P, (Z)-1-(Triphenylsilyl)-2-methylbut-2-ene **438045-65-9P**, (Z)-3-[Dimethyl(phenyl)silylmethyl]-7-methylocta-2,6-**diene** **438045-66-0P**, (E)-2,3-Epoxy-8-[dimethyl(phenyl)silyl]-2,6-dimethyloct-6-ene **438045-67-1P**, (Z)-2,3-Epoxy-6-[dimethyl(phenyl)silylmethyl]-2-methyloct-6-ene **438045-68-2P**, Dimethyl((E)-2-pentenyl)(phenyl)silane **438045-69-3P**, 1-[Dimethyl(phenyl)silyl]pent-2-ene **438045-70-6P**, (2-(2-Cyclohexylethylidene)-6-methyl-5-heptenyl)dimethyl(phenyl)silane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)

IT 438045-60-4P, (1E)-1-Cyclohexyl-7-methyl-3-oxoocta-1,6-**diene**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of)

IT 438045-61-5P, (1E)-1-Cyclohexyl-7-methyl-3-methyleneocta-1,6-**diene**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of)

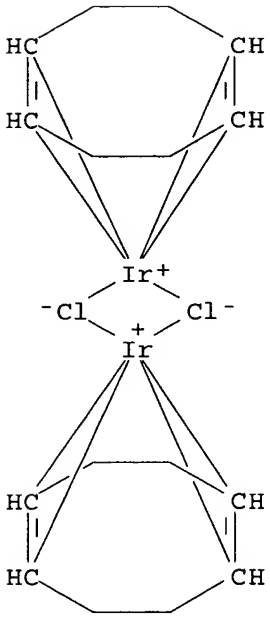
IT 12092-47-6, Bis(chloro(1,5-**cyclooctadiene**)rhodium)
RL: CAT (Catalyst use); USES (Uses)
(with phosphine; effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)

IT 603-35-0, Triphenylphosphine, uses
RL: CAT (Catalyst use); USES (Uses)
(with rhodium chloro **diene** complex; effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)

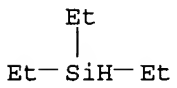
IT **12112-67-3**, Dichlorobis(1,5-**cyclooctadiene**)diiridium
RL: **CAT (Catalyst use)**; USES (Uses)
(effect of oxygen on regioselectivity in catalyzed hydrosilylation of unsym. **diene**)

RN 12112-67-3 HCAPLUS

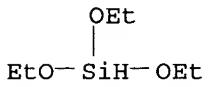
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



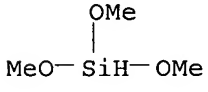
IT **617-86-7**, Triethylsilane **998-30-1**, Triethoxysilane
2487-90-3, Trimethoxysilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)
RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 998-30-1 HCAPLUS
CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 2487-90-3 HCAPLUS
CN Silane, trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

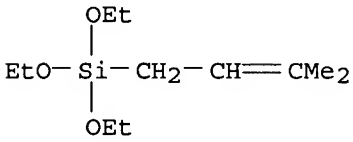


IT **18032-09-2P**, 1-Triethylsilyl-3-methylbut-2-ene **35754-76-8P**
, 1-Triethoxysilyl-3-methylbut-2-ene **50598-99-7P**
63942-83-6P, (Z)-1-Triethoxysilyl-2-methylbut-2-ene

63972-14-5P, 1-[Dimethyl(phenyl)silyl]-3-methylbut-2-ene **68260-36-6P**, (E)-3,7-Dimethyl-1-[dimethyl(phenyl)silyl]octa-2,6-**diene 72142-16-6P**, 1-Trimethoxysilyl-3-methylbut-2-ene **108311-91-7P**, (Z)-1-Triethylsilyl-2-methylbut-2-ene **108311-92-8P**, (Z)-1-Trimethoxysilyl-2-methylbut-2-ene **167314-58-1P**, (Z)-1-[Dimethyl(phenyl)silyl]-2-methylpent-2-ene **438045-62-6P**, (2Z)-1-Cyclohexyl-7-methyl-3-[dimethyl(phenyl)silylmethyl]octa-2,6-**diene 438045-65-9P**, (Z)-3-[Dimethyl(phenyl)silylmethyl]-7-methylocta-2,6-**diene 438045-66-0P**, (E)-2,3-Epoxy-8-[dimethyl(phenyl)silyl]-2,6-dimethyloct-6-ene **438045-67-1P**, (Z)-2,3-Epoxy-6-[dimethyl(phenyl)silylmethyl]-2-methyloct-6-ene **438045-68-2P**, Dimethyl((E)-2-pentenyl)(phenyl)silane **438045-69-3P**, 1-[Dimethyl(phenyl)silyl]pent-2-ene **438045-70-6P**, (2-(2-Cyclohexylethylidene)-6-methyl-5-heptenyl)dimethyl(phenyl)silane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(effect of oxygen on regioselectivity in rhodium catalyzed hydrosilylation of unsym. **diene**)

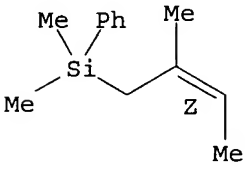
RN 18032-09-2 HCAPLUS
CN Silane, triethyl(3-methyl-2-butenyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

RN 35754-76-8 HCAPLUS
CN Silane, triethoxy(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)



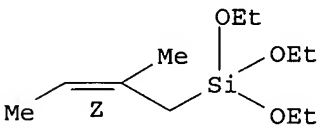
RN 50598-99-7 HCAPLUS
CN Silane, dimethyl[(2Z)-2-methyl-2-butenyl]phenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

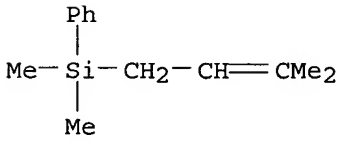


RN 63942-83-6 HCAPLUS
CN Silane, triethoxy[(2Z)-2-methyl-2-butenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

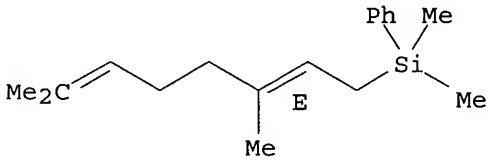


RN 63972-14-5 HCAPLUS
CN Silane, dimethyl(3-methyl-2-butenyl)phenyl- (9CI) (CA INDEX NAME)

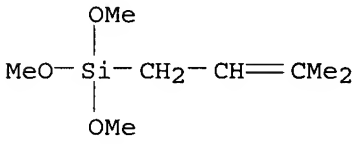


RN 68260-36-6 HCAPLUS
CN Silane, [(2E)-3,7-dimethyl-2,6-octadienyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

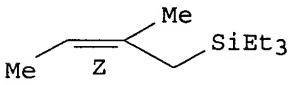


RN 72142-16-6 HCAPLUS
CN Silane, trimethoxy(3-methyl-2-butenyl)- (9CI) (CA INDEX NAME)



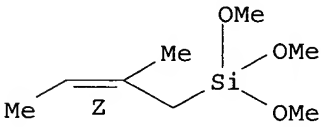
RN 108311-91-7 HCAPLUS
CN Silane, triethyl[(2Z)-2-methyl-2-butenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 108311-92-8 HCAPLUS
CN Silane, trimethoxy[(2Z)-2-methyl-2-butenyl]- (9CI) (CA INDEX NAME)

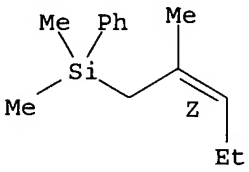
Double bond geometry as shown.



RN 167314-58-1 HCAPLUS

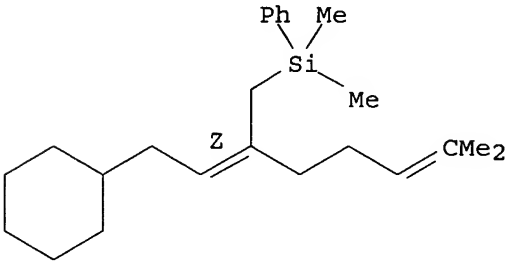
CN Silane, dimethyl[(2Z)-2-methyl-2-pentenyl]phenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



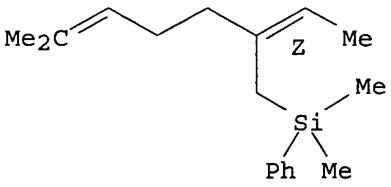
RN 438045-62-6 HCAPLUS
CN Silane, [(2Z)-2-(2-cyclohexylethylidene)-6-methyl-5-heptenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



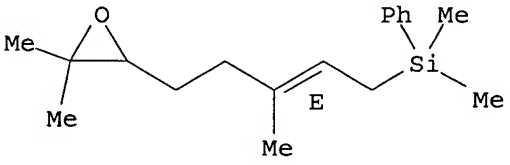
RN 438045-65-9 HCAPLUS
CN Silane, [(2Z)-2-ethylidene-6-methyl-5-heptenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 438045-66-0 HCAPLUS
CN Silane, [(2E)-5-(3,3-dimethyloxiranyl)-3-methyl-2-pentenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

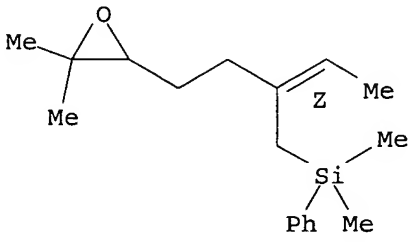
Double bond geometry as shown.



RN 438045-67-1 HCAPLUS
CN Silane, [(2Z)-2-[2-(3,3-dimethyloxiranyl)ethyl]-2-butenyl]dimethylphenyl-

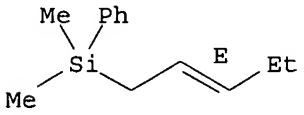
(9CI) (CA INDEX NAME)

Double bond geometry as shown.

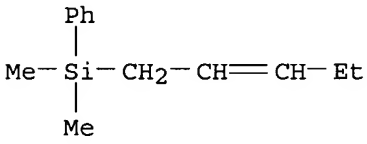


RN 438045-68-2 HCAPLUS
CN Silane, dimethyl-(2E)-2-pentenylphenyl- (9CI) (CA INDEX NAME)

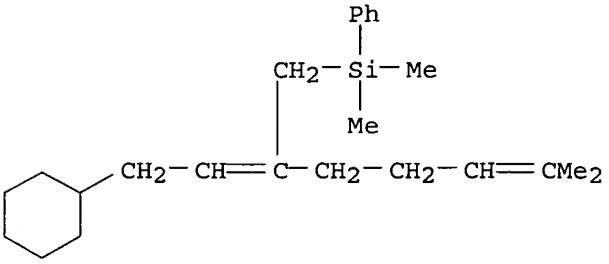
Double bond geometry as shown.



RN 438045-69-3 HCAPLUS
CN Silane, dimethyl-2-pentenylphenyl- (9CI) (CA INDEX NAME)



RN 438045-70-6 HCAPLUS
CN Silane, [2-(2-cyclohexylethylidene)-6-methyl-5-heptenyl]dimethylphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 32 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:128366 HCAPLUS
DOCUMENT NUMBER: 132:251176
TITLE: Dehydrogenative silylation of terminal alkynes by iridium catalyst

AUTHOR(S): Shimizu, Rie; Fuchikami, Takamasa
CORPORATE SOURCE: Sagami Chemical Research Center, Kanagawa, 229-0012, Japan
SOURCE: Tetrahedron Letters (2000), 41(6), 907-910
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dehydrogenative silylation of terminal alkynes with hydrosilanes proceeds in the presence of Ir catalyst to afford the corresponding silylacetylenes. When phenylacetylene and triethylsilane were heated in dry DME in the presence of Ir4(CO)12PPh3, (2-phenylethynyl)triethylsilane was obtained in 96% yield with little of hydrosilylated products. The present method is applicable for a variety of terminal alkynes and hydrosilanes to give the corresponding silylacetylenes in good yields with high selectivities.

CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 603-35-0, Triphenylphosphine, uses **18827-81-1**, Tetrairidium dodecacarbonyl
RL: **CAT (Catalyst use)**; USES (Uses)
(dehydrogenative silylation of terminal alkynes by iridium catalyst)

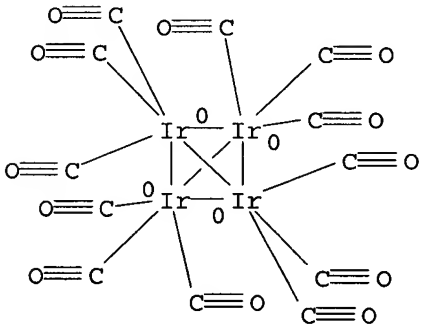
IT 536-74-3, Phenylacetylene **617-86-7**, Triethylsilane 629-05-0, 1-Octyne 766-77-8, Dimethylphenylsilane 917-92-0, 3,3-Dimethyl-1-butyne 931-48-6, Cyclohexylacetylene 1438-82-0, Dimethyl(trimethylsiloxy)silane **14857-34-2**, Ethoxydimethylsilane **29681-57-0**, tert-Butyldimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(dehydrogenative silylation of terminal alkynes by iridium catalyst)

IT 1081-97-6P **4131-43-5P**, Triethyl(phenylethynyl)silane **18408-64-5P**, Triethyl-1-octynylsilane **75573-29-4P** **79628-15-2P**, Dimethylphenyl(phenylethynyl)silane **85443-40-9P**, tert-Butyldimethyl(phenylethynyl)silane **146139-33-5P**, Ethoxydimethyl(phenylethynyl)silane **148991-61-1P**, Cyclohexylethynyltriethylsilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(dehydrogenative silylation of terminal alkynes by iridium catalyst)

IT **18827-81-1**, Tetrairidium dodecacarbonyl
RL: **CAT (Catalyst use)**; USES (Uses)
(dehydrogenative silylation of terminal alkynes by iridium catalyst)

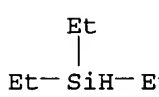
RN 18827-81-1 HCAPLUS

CN Iridium, dodecacarbonyltetra-, tetrahedro (9CI) (CA INDEX NAME)

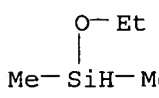


IT **617-86-7**, Triethylsilane **14857-34-2**, Ethoxydimethylsilane **29681-57-0**, tert-Butyldimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**

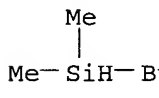
(dehydrogenative silylation of terminal alkynes by iridium catalyst)
RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



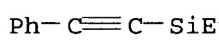
RN 14857-34-2 HCAPLUS
CN Silane, ethoxydimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



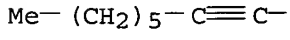
RN 29681-57-0 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)



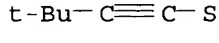
IT **4131-43-5P**, Triethyl(phenylethynyl)silane **18408-64-5P**,
Triethyl-1-octynylsilane **75573-29-4P 79628-15-2P**,
Dimethylphenyl(phenylethynyl)silane **85443-40-9P**,
tert-Butyldimethyl(phenylethynyl)silane **146139-33-5P**,
Ethoxydimethyl(phenylethynyl)silane **148991-61-1P**,
Cyclohexylethynyltriethylsilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(dehydrogenative silylation of terminal alkynes by iridium catalyst)
RN 4131-43-5 HCAPLUS
CN Silane, triethyl(phenylethynyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



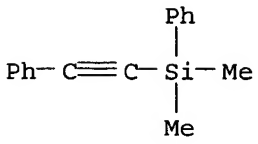
RN 18408-64-5 HCAPLUS
CN Silane, triethyl-1-octynyl- (8CI, 9CI) (CA INDEX NAME)



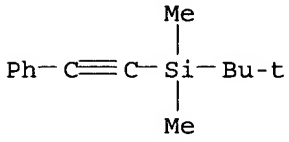
RN 75573-29-4 HCAPLUS
CN Silane, (3,3-dimethyl-1-butynyl)triethyl- (9CI) (CA INDEX NAME)



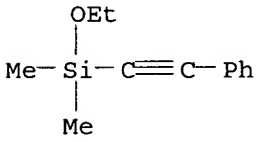
RN 79628-15-2 HCAPLUS
CN Silane, dimethylphenyl(phenylethynyl)- (9CI) (CA INDEX NAME)



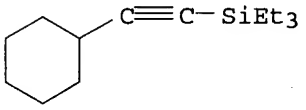
RN 85443-40-9 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 146139-33-5 HCAPLUS
CN Silane, ethoxydimethyl(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 148991-61-1 HCAPLUS
CN Silane, (cyclohexylethynyl)triethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 33 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:377084 HCAPLUS
DOCUMENT NUMBER: 125:58733
TITLE: Process for the preparation of 3-halo- or -pseudohalo-alkylsilane esters
INVENTOR(S): Kropfgans, Frank; Frings, Albert; Horn, Michael; Koetzsch, Hans-Joachim; Monkiewicz, Jaroslaw; Seiler, Claus-Dietrich; Srebny, Hans-Guenther; Standke, Burkhard
PATENT ASSIGNEE(S): Huels Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 709392	A1	19960501	EP 1995-113741	19950901
EP 709392	B1	20010516		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
DE 19534853	A1	19960502	DE 1995-19534853	19950920
CA 2161181	AA	19960426	CA 1995-2161181	19951023
JP 08208667	A2	19960813	JP 1995-275580	19951024
US 5616762	A	19970401	US 1995-548131	19951025
PRIORITY APPLN. INFO.:			DE 1994-4438031 A	19941025
			DE 1995-19534853 A	19950920

OTHER SOURCE(S): CASREACT 125:58733; MARPAT 125:58733

AB The preparation of title compds., XCR2R3CHR1CH2SiRn(OR4)3-n (R = C1-18 alkyl or cycloalkyl, halo; R1 = H, R; R2 = H, R, substituted aryl, halo; R3 = same or different R2; R3 = C1-10 alkyl, aliphatic ether containing group; X = F, Cl, Br, iodo, cyano, isocyanato, isothiocyanato, azido; n = 0-2) via iridium catalyzed hydrosilylation of XCR2R3CR1:CH2 with HSiRn(OR4)3-n is described. Thus, IrCl3 hydrate catalyzed hydrosilylation of allyl chloride with triethoxysilane in 3-chloropropyltriethoxysilane as reaction medium gave 86% 3-chloropropyltriethoxysilane.

IC ICM C07F007-18

CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 78-10-4P, Tetraethoxysilane **2031-67-6P**, Methyltriethoxysilane **2550-02-9P**, Propyltriethoxysilane **177951-95-0P**, Isobutyldiethoxymethylsilane
RL: BYP (Byproduct); **PREP (Preparation)**
(preparation of)

IT **5089-70-3P**, 3-Chloropropyltriethoxysilane **24801-88-5P**, 3-Isocyanatopropyltriethoxysilane **122055-02-1P**, (3-Isothiocyanatopropyl)trimethoxysilane **177951-94-9P**, (3-Chloroisobutyl)diethoxymethylsilane **177951-96-1P**, Cyclopentyldiethoxy(3,3,3-trifluoropropyl)silane **177951-97-2P**, 3-Bromopropyl(2-butoxyethoxy)dimethylsilane **177951-98-3P**, (3,4-Dichloro-2-methylbutyl)ethyldimethoxysilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

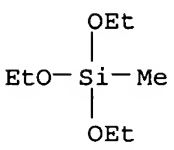
IT **12112-67-3**, Chloro(1,5-**cyclooctadiene**)iridium dimer 14996-61-3, Iridium trichloride hydrate 16941-92-7, Dihydrogen hexachloroiridate **51812-37-4**, Carbonylchlorobis(**cyclooctadiene**)iridium dimer
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of halo or pseudohalo substituted alkylsilane esters via iridium catalyzed hydrosilylation of unsatd. compds. with alkoxysilanes)

IT 57-06-7 106-95-6, Allyl bromide, reactions 107-05-1, Allyl chloride 563-47-3, Methallyl chloride 677-21-4, 3,3,3-Trifluoro-1-propene **998-30-1**, Triethoxysilane 1476-23-9, Allyl isocyanate **2031-62-1**, Methyldiethoxysilane **2487-90-3**, Trimethoxysilane **19753-84-5**, Ethyldimethoxysilane 53920-89-1 177951-92-7, Cyclopentyldiethoxysilane **177951-93-8**, (2-Butoxyethoxy)dimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of halo or pseudohalo substituted alkylsilane esters via iridium catalyzed hydrosilylation of unsatd. compds. with alkoxysilanes)

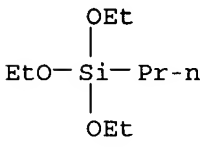
IT **2031-67-6P**, Methyltriethoxysilane **2550-02-9P**, Propyltriethoxysilane **177951-95-0P**, Isobutyldiethoxymethylsilane
RL: BYP (Byproduct); **PREP (Preparation)**
(preparation of)

RN 2031-67-6 HCAPLUS

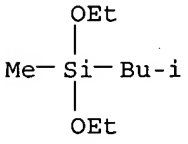
CN Silane, triethoxymethyl- (8CI, 9CI) (CA INDEX NAME)



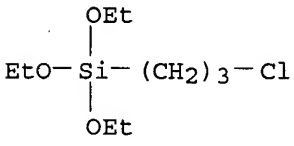
RN 2550-02-9 HCAPLUS
CN Silane, triethoxypropyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



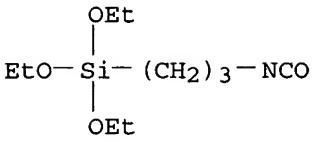
RN 177951-95-0 HCAPLUS
CN Silane, diethoxymethyl(2-methylpropyl)- (9CI) (CA INDEX NAME)



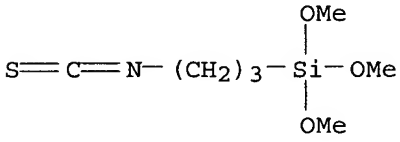
IT **5089-70-3P**, 3-Chloropropyltriethoxysilane **24801-88-5P**,
3-Isocyanatopropyltriethoxysilane **122055-02-1P**,
(3-Isothiocyanatopropyl)trimethoxysilane **177951-94-9P**,
(3-Chloroisobutyl)diethoxymethylsilane **177951-96-1P**,
Cyclopentyldiethoxy(3,3,3-trifluoropropyl)silane **177951-97-2P**,
3-Bromopropyl(2-butoxyethoxy)dimethylsilane **177951-98-3P**,
(3,4-Dichloro-2-methylbutyl)ethyldimethoxysilane
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 5089-70-3 HCAPLUS
CN Silane, (3-chloropropyl)triethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



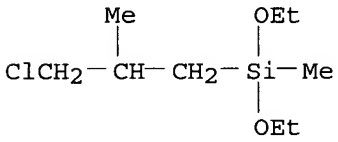
RN 24801-88-5 HCAPLUS
CN Silane, triethoxy(3-isocyanatopropyl)- (9CI) (CA INDEX NAME)



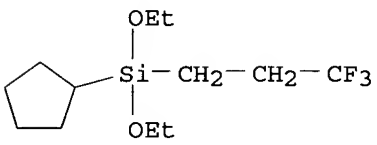
RN 122055-02-1 HCAPLUS
CN Silane, (3-isothiocyanatopropyl)trimethoxy- (9CI) (CA INDEX NAME)



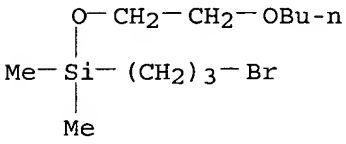
RN 177951-94-9 HCAPLUS
CN Silane, (3-chloro-2-methylpropyl)diethoxymethyl- (9CI) (CA INDEX NAME)



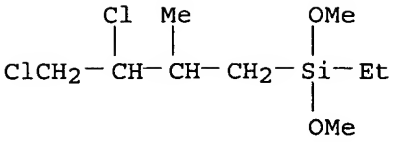
RN 177951-96-1 HCAPLUS
CN Silane, cyclopentyldiethoxy(3,3,3-trifluoropropyl)- (9CI) (CA INDEX NAME)



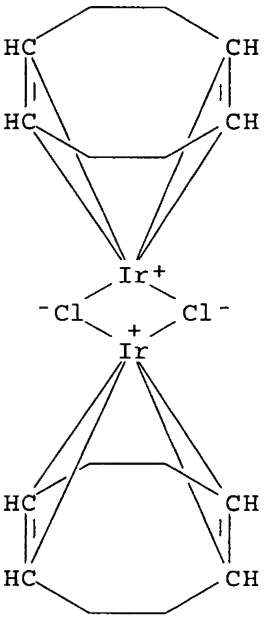
RN 177951-97-2 HCAPLUS
CN Silane, (3-bromopropyl)(2-butoxyethoxy)dimethyl- (9CI) (CA INDEX NAME)



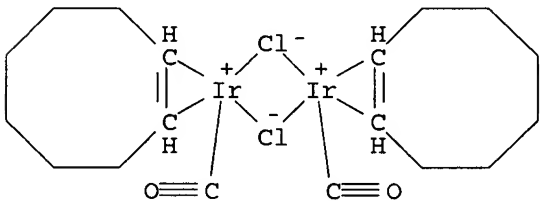
RN 177951-98-3 HCAPLUS
CN Silane, (3,4-dichloro-2-methylbutyl)ethyldimethoxy- (9CI) (CA INDEX NAME)



IT **12112-67-3**, Chloro(1,5-**cyclooctadiene**)iridium dimer
51812-37-4, Carbonylchlorobis(**cyclooctadiene**)iridium dimer
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of halo or pseudohalo substituted alkylsilane esters via iridium catalyzed hydrosilylation of unsatd. compds. with alkoxysilanes)
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



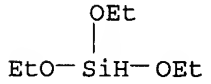
RN 51812-37-4 HCAPLUS
CN Iridium, dicarbonyldi-μ-chlorobis[(1,2-η)-cyclooctene]di- (9CI) (CA INDEX NAME)



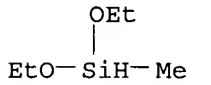
IT **998-30-1**, Triethoxysilane **2031-62-1**, Methyldiethoxysilane **2487-90-3**, Trimethoxysilane

19753-84-5, Ethyldimethoxysilane **177951-93-8**,
(2-Butoxyethoxy)dimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of halo or pseudohalo substituted alkylsilane esters via iridium catalyzed hydrosilylation of unsatd. compds. with alkoxysilanes)

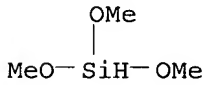
RN 998-30-1 HCAPLUS
CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)



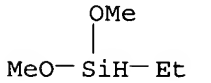
RN 2031-62-1 HCAPLUS
CN Silane, diethoxymethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



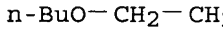
RN 2487-90-3 HCAPLUS
CN Silane, trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 19753-84-5 HCAPLUS
CN Silane, ethyldimethoxy- (8CI, 9CI) (CA INDEX NAME)

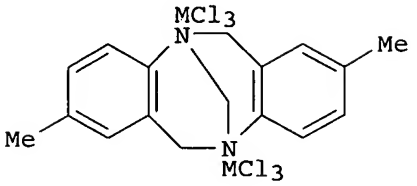


RN 177951-93-8 HCAPLUS
CN Silane, (2-butoxyethoxy)dimethyl- (9CI) (CA INDEX NAME)



L64 ANSWER 34 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:316883 HCAPLUS
DOCUMENT NUMBER: 122:160759
TITLE: Transition metal complexes of Troeger's base and their catalytic activity for the hydrosilylation of alkynes
AUTHOR(S): Goldberg, Yuri; Alper, Howard
CORPORATE SOURCE: Department Chemistry, University Ottawa, Ottawa, ON, K1N 6N5, Can.
SOURCE: Tetrahedron Letters (1995), 36(3), 369-72
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:160759
GI



I

AB Rhodium(III) and iridium(III) complexes of Troger's base (TB), of structural type I (M = Rh, Ir), were prepared by treatment of TB with MCl3. The rhodium complex readily catalyzed the hydrosilylation of alkynes with high regio- and stereoselectivity observed in some cases.

CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 78

IT **3412-58-6P 3412-59-7P 21209-32-5P**
42478-41-1P 61518-55-6P 64545-09-1P
64545-10-4P 64788-84-7P 64788-85-8P
75645-33-9P 76372-98-0P 109681-42-7P
130613-30-8P 130613-31-9P 144967-38-4P
160424-09-9P 160424-10-2P 161403-16-3P
161403-17-4P 161403-18-5P 161403-19-6P
161403-20-9P 161403-21-0P 161403-22-1P
161403-23-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

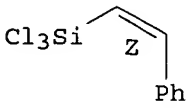
IT 161377-10-2P **161377-11-3P** 161444-29-7P 161444-30-0P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(transition metal complexes of Troeger's base and catalytic activity for hydrosilylation of alkynes)

IT 536-74-3, Phenylacetylene **617-86-7**, Triethylsilane 693-02-7, 1-Hexyne 766-77-8, Dimethylphenylsilane **1066-35-9**, Chlorodimethylsilane **6485-79-6**, Triisopropylsilane **10025-78-2**, Trichlorosilane 14267-92-6 **29681-57-0**, tert-Butyldimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(transition metal complexes of Troeger's base and catalytic activity for hydrosilylation of alkynes)

IT **3412-58-6P 3412-59-7P 21209-32-5P**
42478-41-1P 61518-55-6P 64545-09-1P
64545-10-4P 64788-84-7P 64788-85-8P
75645-33-9P 76372-98-0P 109681-42-7P
130613-30-8P 130613-31-9P 144967-38-4P
160424-09-9P 160424-10-2P 161403-16-3P
161403-17-4P 161403-18-5P 161403-19-6P
161403-20-9P 161403-21-0P 161403-22-1P
161403-23-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

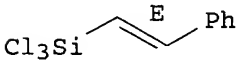
RN 3412-58-6 HCAPLUS
CN Silane, trichloro[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



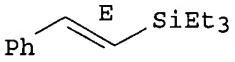
RN 3412-59-7 HCAPLUS
CN Silane, trichloro[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

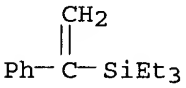


RN 21209-32-5 HCAPLUS
CN Silane, triethyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

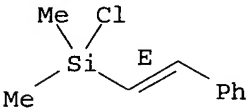


RN 42478-41-1 HCAPLUS
CN Silane, triethyl(1-phenylethenyl)- (9CI) (CA INDEX NAME)



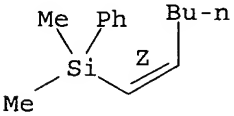
RN 61518-55-6 HCAPLUS
CN Silane, chlorodimethyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



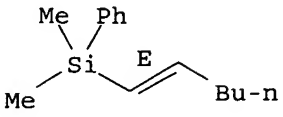
RN 64545-09-1 HCAPLUS
CN Silane, (1Z)-1-hexenyldimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



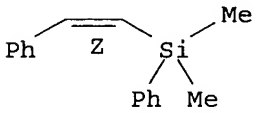
RN 64545-10-4 HCAPLUS
CN Silane, (1E)-1-hexenyldimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



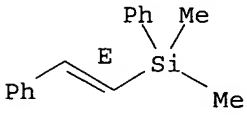
RN 64788-84-7 HCAPLUS
CN Silane, dimethylphenyl[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



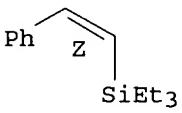
RN 64788-85-8 HCAPLUS
CN Silane, dimethylphenyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



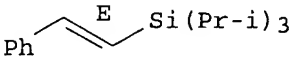
RN 75645-33-9 HCAPLUS
CN Silane, triethyl[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

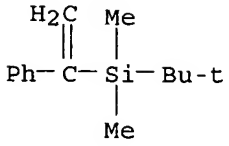


RN 76372-98-0 HCAPLUS
CN Silane, tris(1-methylethyl)(2-phenylethenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

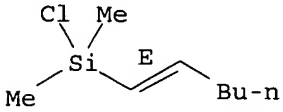


RN 109681-42-7 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl(1-phenylethenyl)- (9CI) (CA INDEX NAME)

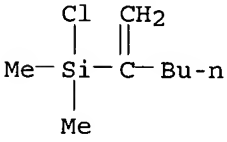


RN 130613-30-8 HCAPLUS
CN Silane, chloro-(1E)-1-hexenyldimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

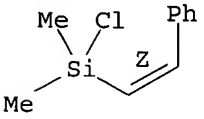


RN 130613-31-9 HCAPLUS
CN Silane, chlorodimethyl(1-methylenepentyl)- (9CI) (CA INDEX NAME)



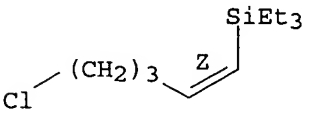
RN 144967-38-4 HCAPLUS
CN Silane, chlorodimethyl[(1Z)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



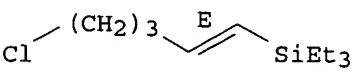
RN 160424-09-9 HCAPLUS
CN Silane, (5-chloro-1-pentenyl)triethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



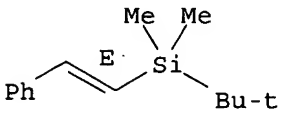
RN 160424-10-2 HCAPLUS
CN Silane, [(1E)-5-chloro-1-pentenyl]triethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

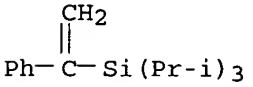


RN 161403-16-3 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[(1E)-2-phenylethenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

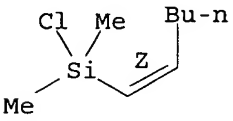


RN 161403-17-4 HCAPLUS
CN Silane, tris(1-methylethyl)(1-phenylethenyl)- (9CI) (CA INDEX NAME)



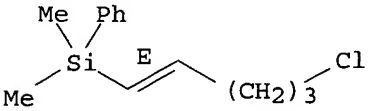
RN 161403-18-5 HCAPLUS
CN Silane, chloro-1-hexenyldimethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



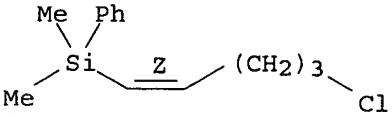
RN 161403-19-6 HCAPLUS
CN Silane, [(1E)-5-chloro-1-pentenyl]dimethylphenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



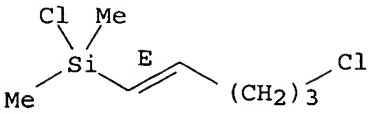
RN 161403-20-9 HCAPLUS
CN Silane, (5-chloro-1-pentenyl)dimethylphenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



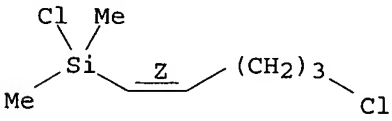
RN 161403-21-0 HCAPLUS
CN Silane, chloro(5-chloro-1-pentenyl)dimethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

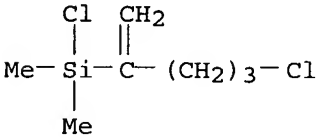


RN 161403-22-1 HCAPLUS
CN Silane, chloro(5-chloro-1-pentenyl)dimethyl-, (Z)- (9CI) (CA INDEX NAME)

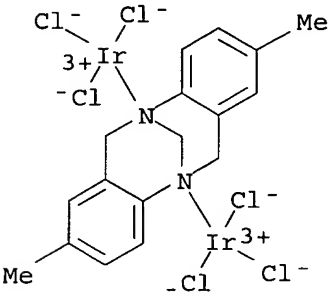
Double bond geometry as shown.



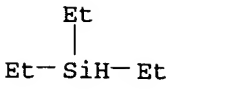
RN 161403-23-2 HCAPLUS
CN Silane, chloro(4-chloro-1-methylenebutyl)dimethyl- (9CI) (CA INDEX NAME)



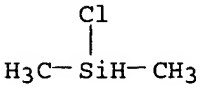
IT **161377-11-3P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(transition metal complexes of Troeger's base and catalytic activity for hydrosilylation of alkynes)
RN 161377-11-3 HCAPLUS
CN Iridium, hexachloro[μ-(2,8-dimethyl-6H,12H-5,11-methanodibenzo[b,f][1,5]diazocine-N5:N11)]di- (9CI) (CA INDEX NAME)



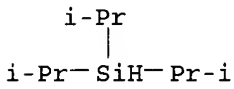
IT **617-86-7**, Triethylsilane **1066-35-9**, Chlorodimethylsilane **6485-79-6**, Triisopropylsilane **10025-78-2**, Trichlorosilane **29681-57-0**, tert-Butyldimethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(transition metal complexes of Troeger's base and catalytic activity for hydrosilylation of alkynes)
RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



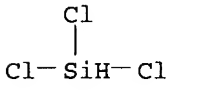
RN 1066-35-9 HCAPLUS
CN Silane, chlorodimethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



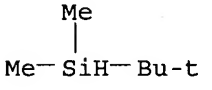
RN 6485-79-6 HCAPLUS
CN Silane, tris(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 10025-78-2 HCAPLUS
CN Silane, trichloro- (8CI, 9CI) (CA INDEX NAME)



RN 29681-57-0 HCAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

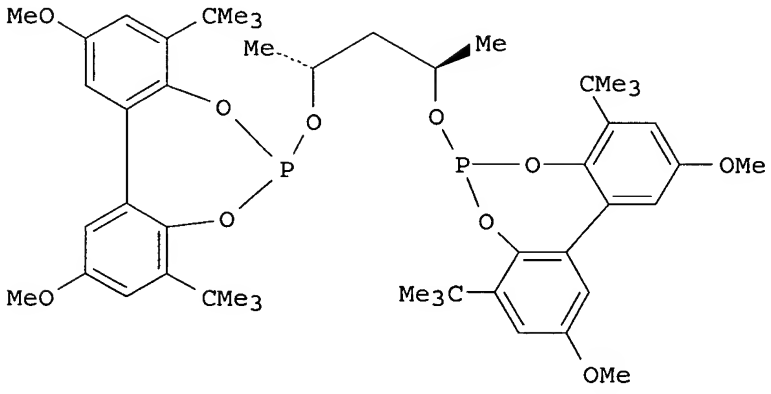


L64 ANSWER 35 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:229480 HCAPLUS
DOCUMENT NUMBER: 122:186609
TITLE: Asymmetric syntheses using optically active metal-ligand complex catalysts
INVENTOR(S): Babin, James E.; Whiteker, Gregory T.
PATENT ASSIGNEE(S): Union Carbide Chemicals and Plastics Technology Corp., USA
SOURCE: U.S., 23 pp. Cont.-in-part of U.S. Ser. No. 748,112. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 5360938	A	19941101	US 1992-911518		19920716
IL 102873	A1	20010520	IL 1992-102873		19920819
ZA 9206289	A	19930303	ZA 1992-6289		19920820
WO 9303839	A1	19930304	WO 1992-US6808		19920820
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, PL, RO, RU, SD					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG					
AU 9225077	A1	19930316	AU 1992-25077		19920820
CN 1071431	A	19930428	CN 1992-110864		19920820
CN 1038938	B	19980701			
EP 600020	A1	19940608	EP 1992-919034		19920820
EP 600020	B1	19960131			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE					
IN 174153	A	19940924	IN 1992-MA516		19920820
BR 9206391	A	19950301	BR 1992-6391		19920820
AT 133584	E	19960215	AT 1992-919034		19920820
ES 2085644	T3	19960601	ES 1992-919034		19920820
CA 2116098	C	19980120	CA 1992-2116098		19920820
KR 136357	B1	19980425	KR 1994-700550		19940221
IN 178002	A	19970301	IN 1994-MA313		19940420
US 5491266	A	19960213	US 1994-262508		19940620
PRIORITY APPLN. INFO.:			US 1991-748111	B2	19910821
			US 1991-748112	A2	19910821
			US 1992-911518	A	19920716
			IN 1992-MA516	A1	19920820
			WO 1992-US6808	A	19920820

OTHER SOURCE(S): MARPAT 122:186609
GI



I

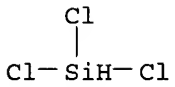
AB This invention relates to asym. syntheses in which a prochiral or chiral compound is contacted in the presence of an optically active metal-ligand complex catalyst to produce an optically active product. Thus, e.g., asym. hydroformylation of styrene with a catalyst solution containing rhodium dicarbonyl acetylacetonate and ligand I afforded an isomer ratio of 12.4:1 (2-phenylpropionaldehyde:hydrocinnamaldehyde); oxidation of the product aldehydes afforded an 80:20 ratio of the S and R enantiomers of 2-phenylpropionic acid.

IC ICM C07C045-00
INCL 568449000

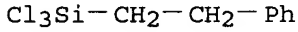
CC 21-2 (General Organic Chemistry)
IT 1295-35-8, Bis(1,5-**cyclooctadiene**)nickel(0) 7439-88-5D, Iridium, optically active ligand complexes 7439-89-6D, Iron, optically active ligand complexes 7440-02-0D, Nickel, optically active ligand complexes 7440-04-2D, Osmium, optically active ligand complexes 7440-05-3D, Palladium, optically active ligand complexes 7440-06-4D, Platinum, optically active ligand complexes 7440-16-6D, Rhodium, optically active ligand complexes 7440-18-8D, Ruthenium, optically active ligand complexes 7440-48-4D, Cobalt, optically active ligand complexes 7758-89-6, Copper(I) chloride **12111-11-4**, Bicyclo[2.2.1]hepta-2,5-**dieneiridium**(I) chloride dimer 14284-93-6 14874-82-9, Rhodium dicarbonyl acetylacetonate 38816-56-7, Bis(bicyclo[2.2.1]hepta-2,5-**diene**)rhodium(I) hexafluorophosphate 60576-58-1, Bis(bicyclo[2.2.1]hepta-2,5-**diene**)rhodium(I) perchlorate 90243-59-7, cis-Dichlorobis(acetonitrile)palladium(II)
RL: **CAT (Catalyst use)**; USES (Uses)
(asym. synthesis using optically active metal-ligand complex catalysts)
IT 97-65-4, Itaconic Acid, reactions 98-83-9, α-Methylstyrene, reactions 98-86-2, Acetophenone, reactions 100-42-5, Styrene, reactions 100-52-7, Benzaldehyde, reactions 108-05-4, Vinyl Acetate, reactions 128-37-0, 2,6-Di-tert-butyl-4-methylphenol, reactions 498-66-8, Norbornene 592-41-6, 1-Hexene, reactions 1079-66-9, Chlorodiphenylphosphine **10025-78-2**, Trichlorosilane 16611-68-0 18531-94-7 18531-99-2, (S)-1,1'-Bi-2-naphthol 31469-15-5, Methyl trimethylsilyl dimethylketene acetal 42075-32-1, (2R,4R)-Pentanediol 63444-51-9, 6-Methoxy-2-vinylnaphthalene 63444-56-4, p-Isobutylstyrene 71941-98-5 72345-23-4, (2S,4S)-Pentanediol 73346-74-4, (-)-2,3-O-Isopropylidene-D-threitol 82017-87-6 108609-95-6 134170-23-3 137156-22-0
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(asym. synthesis using optically active metal-ligand complex catalysts)
IT **940-41-0P**, 2-Trichlorosilylethylbenzene 32305-59-2P 33530-47-1P, (S)-2-Phenylpropionaldehyde 38235-74-4P, (R)-2-Phenylpropionaldehyde 56800-48-7P 110773-62-1P 114937-27-8P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(asym. synthesis using optically active metal-ligand complex catalysts)
IT 60-12-8P, 2-Phenylethanol 111-71-7P, n-Heptanal 645-59-0P, Hydrocinnamonitrile 939-90-2P 1445-91-6P 1517-69-7P 2174-58-5P 2234-26-6P, 2-Norbornanecarbonitrile 3641-51-8P 7782-24-3P, (S)-2-Phenylpropionic acid 7782-26-5P, (R)-2-Phenylpropionic acid **13340-46-0P**, 2-Triethoxysilylethylbenzene 22204-53-1P 23020-18-0P 42307-58-4P, (R)-3-Phenylbutyraldehyde 42412-76-0P 48126-51-8P 51146-56-6P 53531-19-4P, (S)-3-Phenylbutyraldehyde 55630-27-8P 60933-33-7P 66875-69-2P, (R)-α-Acetoxypropanal 66875-70-5P, (S)-α-Acetoxypropanal 66875-71-6P, (S)-2-Methylhexanal 79201-73-3P 104418-69-1P 110849-52-0P 132151-88-3P, (R)-2-Methylhexanal **159909-89-4P** **159909-90-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(asym. synthesis using optically active metal-ligand complex catalysts)
IT **12111-11-4**, Bicyclo[2.2.1]hepta-2,5-**dieneiridium**(I) chloride dimer
RL: **CAT (Catalyst use)**; USES (Uses)
(asym. synthesis using optically active metal-ligand complex catalysts)
RN 12111-11-4 HCAPLUS
CN Iridium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

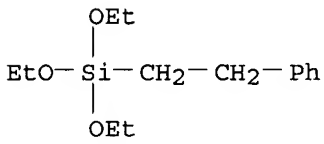
IT **10025-78-2**, Trichlorosilane
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(asym. synthesis using optically active metal-ligand complex catalysts)
RN 10025-78-2 HCAPLUS
CN Silane, trichloro- (8CI, 9CI) (CA INDEX NAME)



IT **940-41-0P**, 2-Trichlorosilylethylbenzene
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(asym. synthesis using optically active metal-ligand complex catalysts)
RN 940-41-0 HCAPLUS
CN Silane, trichloro(2-phenylethyl)- (9CI) (CA INDEX NAME)

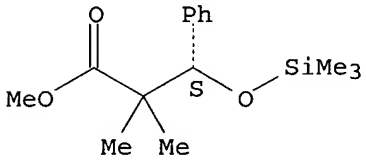


IT **13340-46-0P**, 2-Triethoxysilylethylbenzene **159909-89-4P** **159909-90-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(asym. synthesis using optically active metal-ligand complex catalysts)
RN 13340-46-0 HCAPLUS
CN Silane, triethoxy(2-phenylethyl)- (9CI) (CA INDEX NAME)



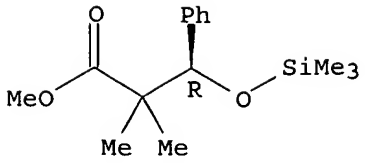
RN 159909-89-4 HCAPLUS
CN Benzenepropanoic acid, α,α-dimethyl-β-[(trimethylsilyl)oxy]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 159909-90-7 HCAPLUS
CN Benzenepropanoic acid, α,α-dimethyl-β-[(trimethylsilyl)oxy]-, methyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L64 ANSWER 36 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:651413 HCAPLUS
DOCUMENT NUMBER: 117:251413
TITLE: Conversion of **alkenes** to enol silyl ethers of acylsilanes by iridium-catalyzed reaction with a hydrosilane and carbon monoxide
AUTHOR(S): Chatani, Naoto; Ikeda, Shinichi; Ohe, Kouichi; Murai, Shinji
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, 565, Japan
SOURCE: Journal of the American Chemical Society (1992), 114(24), 9710-11
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:251413

AB The reaction of **alkenes**, e.g., RCH:CH2 (R = Bu, cyclohexyl, Me3C, etc.; 5-10 equiv, 14 examples) with a hydrosilane (1 equiv, HSiEt2Me, HSiEt3, HSiPhMe2) and CO (50 atm) in the presence of an iridium complex (0.02 equiv, [IrCl(CO)3]n, Ir4(CO)12) at 140° in benzene resulted in the incorporation of CO to give an E/Z mixture of 1-silyl enol silyl ethers, RCH2CH:C(SiR13)(OSiR13) (II) in 45-85% yields. II can be easily hydrolyzed to acylsilanes, e.g. BuCH2CH2COSiEt2Me, (acetone/HCl (0.2 M) = 4/1 at 25°). The overall transformation is a novel, unique method for the preparation of acylsilanes from **alkenes.**

CC 29-6 (Organometallic and Organometalloidal Compounds)
ST **alkene** hydrosilylation iridium catalyzed carbon monoxide; regiochem iridium catalyzed hydrosilylation **alkene**; enol silyl ether prepn hydrolysis; acylsilane
IT **Alkenes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrosilylation of, in presence of carbon monoxide, iridium-catalyzed, enol silyl ethers by)
IT Hydrosilylation catalysts
(iridium complexes, for **alkenes** in presence of carbon monoxide, enol silyl ethers by)
IT Hydrosilylation
(of **alkenes** in presence of carbon monoxide, enol silyl ethers by)
IT Regiochemistry
(of hydrosilylation of **alkenes** with hydrosilanes in presence of carbon monoxide, enol silyl ethers by)
IT Ethers, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(enol, silyl, preparation of, by iridium-catalyzed hydrosilylation of **alkenes** in presence of carbon monoxide)
IT **18827-81-1** 32594-40-4
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for iridium-catalyzed hydrosilylation of **alkenes** with hydrosilanes in presence of carbon monoxide)
IT **617-86-7**, Triethylsilane **760-32-7**, Methyldiethylsilane

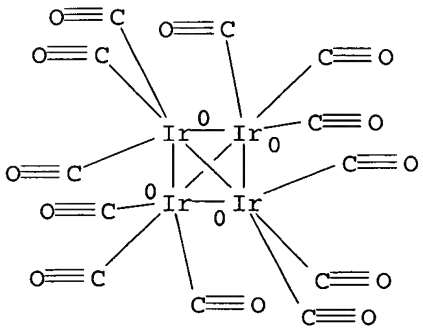
766-77-8, Dimethylphenylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrosilylation by, of **alkenes** in presence of carbon monoxide, iridium-catalyzed, enol silyl ether by)

IT **144542-05-2P 144542-06-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of, acylsilane by)

IT **144542-07-4P 144542-08-5P 144542-09-6P**
144542-10-9P 144542-11-0P 144542-12-1P
144542-13-2P 144542-14-3P 144542-15-4P
144542-16-5P 144542-17-6P 144542-18-7P
144542-19-8P 144542-20-1P 144542-21-2P
144542-22-3P 144542-23-4P 144542-24-5P
144542-25-6P 144542-26-7P 144542-27-8P
144542-28-9P 144542-29-0P 144542-30-3P
144542-31-4P 144542-32-5P 144542-33-6P
144542-34-7P 144542-35-8P 144564-72-7P
144564-73-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)

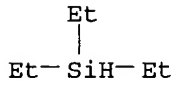
IT **18827-81-1**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for iridium-catalyzed hydrosilylation of **alkenes** with hydrosilanes in presence of carbon monoxide)

RN 18827-81-1 HCAPLUS
CN Iridium, dodecacarbonyltetra-, tetrahedro (9CI) (CA INDEX NAME)

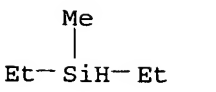


IT **617-86-7**, Triethylsilane **760-32-7**, Methyldiethylsilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrosilylation by, of **alkenes** in presence of carbon monoxide, iridium-catalyzed, enol silyl ether by)

RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)

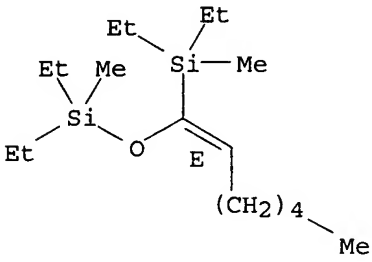


RN 760-32-7 HCAPLUS
CN Silane, diethylmethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



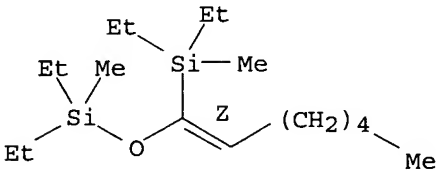
IT **144542-05-2P 144542-06-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of, acylsilane by)
RN 144542-05-2 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-1-heptenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



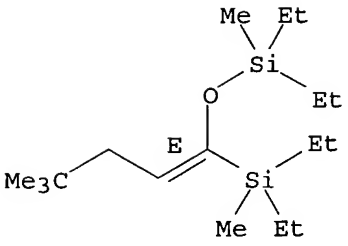
RN 144542-06-3 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-1-heptenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



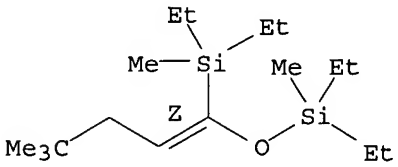
IT **144542-07-4P 144542-08-5P 144542-09-6P**
144542-10-9P 144542-11-0P 144542-12-1P
144542-13-2P 144542-14-3P 144542-15-4P
144542-16-5P 144542-17-6P 144542-18-7P
144542-19-8P 144542-20-1P 144542-21-2P
144542-22-3P 144542-23-4P 144542-24-5P
144542-25-6P 144542-26-7P 144542-27-8P
144542-28-9P 144542-29-0P 144542-30-3P
144542-31-4P 144542-32-5P 144542-33-6P
144542-34-7P 144542-35-8P 144564-72-7P
144564-73-8P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 144542-07-4 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-4,4-dimethyl-1-pentenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



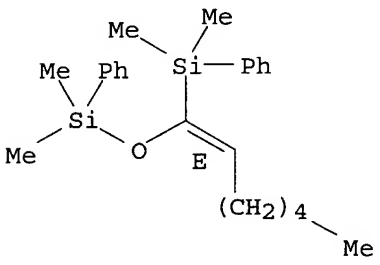
RN 144542-08-5 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-4,4-dimethyl-1-pentenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



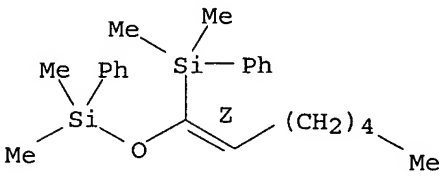
RN 144542-09-6 HCAPLUS
CN Silane, [[1-(dimethylphenylsilyl)-1-heptenyl]oxy]dimethylphenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



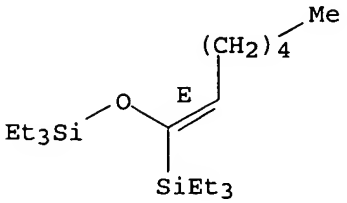
RN 144542-10-9 HCAPLUS
CN Silane, [[1-(dimethylphenylsilyl)-1-heptenyl]oxy]dimethylphenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



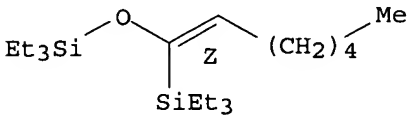
RN 144542-11-0 HCAPLUS
CN Silane, triethyl[[1-(triethylsilyl)-1-heptenyl]oxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



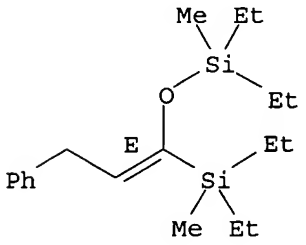
RN 144542-12-1 HCAPLUS
CN Silane, triethyl[[1-(triethylsilyl)-1-heptenyl]oxy]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



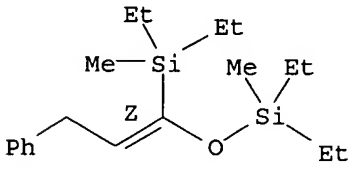
RN 144542-13-2 HCAPLUS
CN Silane, [1-[(diethylmethylsilyl)oxy]-3-phenyl-1-propenyl]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



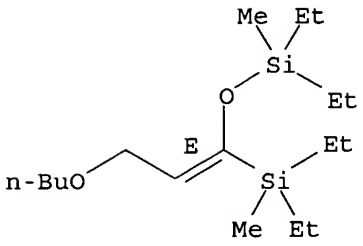
RN 144542-14-3 HCAPLUS
CN Silane, [1-[(diethylmethylsilyl)oxy]-3-phenyl-1-propenyl]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



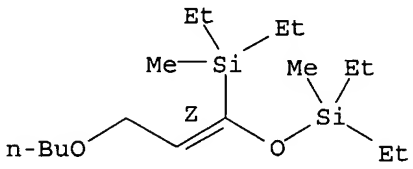
RN 144542-15-4 HCAPLUS
CN Silane, [3-butoxy-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



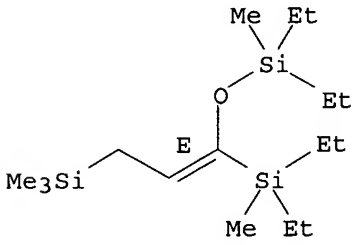
RN 144542-16-5 HCAPLUS
CN Silane, [3-butoxy-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



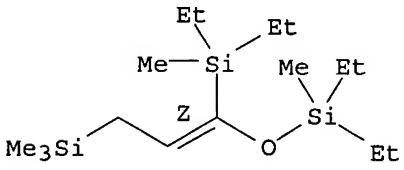
RN 144542-17-6 HCAPLUS
CN Silane, [3-(diethylmethylsilyl)-3-[(diethylmethylsilyl)oxy]-2-propenyl]trimethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



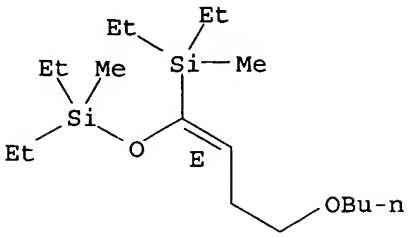
RN 144542-18-7 HCAPLUS
CN Silane, [3-(diethylmethylsilyl)-3-[(diethylmethylsilyl)oxy]-2-propenyl]trimethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



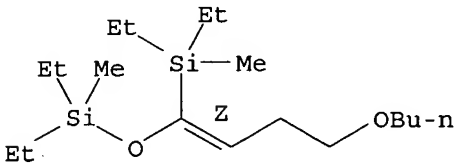
RN 144542-19-8 HCAPLUS
CN Silane, [[4-butoxy-1-(diethylmethylsilyl)-1-butenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



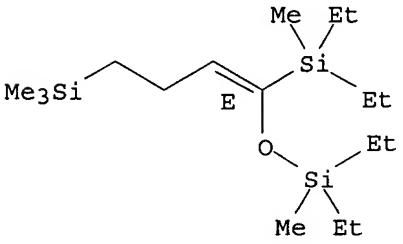
RN 144542-20-1 HCAPLUS
CN Silane, [[4-butoxy-1-(diethylmethylsilyl)-1-butenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



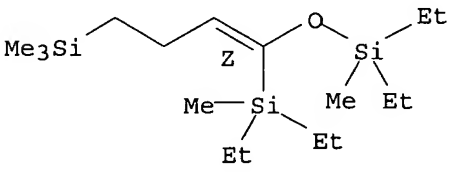
RN 144542-21-2 HCAPLUS
CN Silane, [4-(diethylmethylsilyl)-4-[(diethylmethylsilyl)oxy]-3-butenyl]trimethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 144542-22-3 HCAPLUS
CN Silane, [4-(diethylmethylsilyl)-4-[(diethylmethylsilyl)oxy]-3-butenyl]trimethyl-, (Z)- (9CI) (CA INDEX NAME)

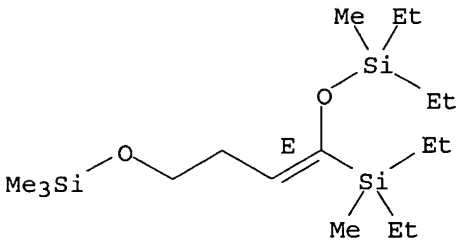
Double bond geometry as shown.



RN 144542-23-4 HCAPLUS
CN 3,8-Dioxa-2,9-disilaundec-6-ene, 7-(diethylmethylsilyl)-9-ethyl-2,2,9-

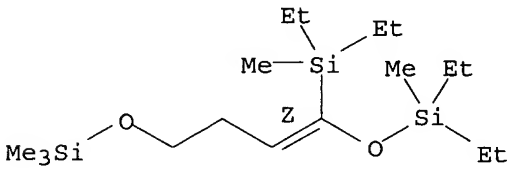
trimethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



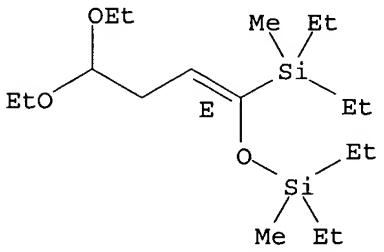
RN 144542-24-5 HCAPLUS
CN 3,8-Dioxa-2,9-disilaundec-6-ene, 7-(diethylmethylsilyl)-9-ethyl-2,2,9-trimethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



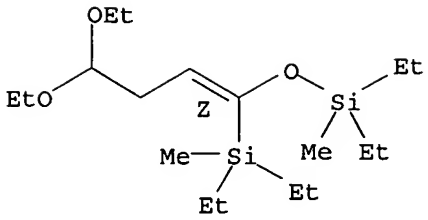
RN 144542-25-6 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-4,4-diethoxy-1-butenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



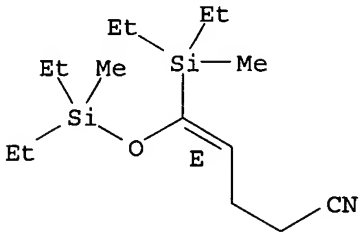
RN 144542-26-7 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-4,4-diethoxy-1-butenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



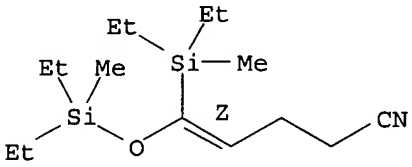
RN 144542-27-8 HCAPLUS
CN 4-Pentenenitrile, 5-(diethylmethylsilyl)-5-[(diethylmethylsilyl)oxy]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



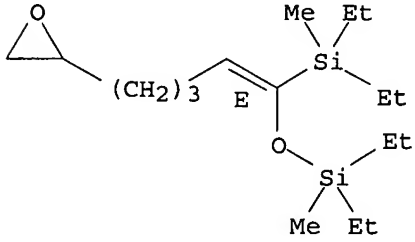
RN 144542-28-9 HCAPLUS
CN 4-Pentenenitrile, 5-(diethylmethylsilyl)-5-[(diethylmethylsilyl)oxy]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 144542-29-0 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-5-oxiranyl-1-pentenyl]oxy]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

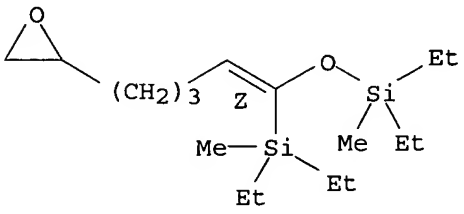
Double bond geometry as shown.



RN 144542-30-3 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-5-oxiranyl-1-pentenyl]oxy]diethylmethyl-,

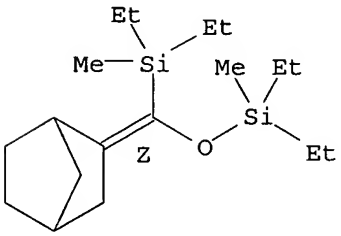
(Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



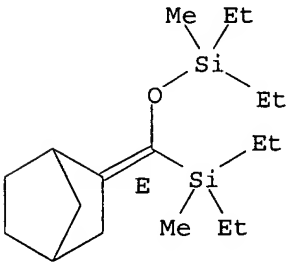
RN 144542-31-4 HCAPLUS
CN Silane, [bicyclo[2.2.1]hept-2-ylidene(diethylmethylsilyl)methoxy]diethylme
thyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



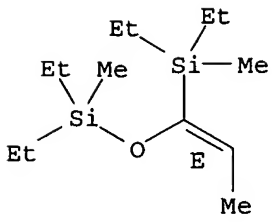
RN 144542-32-5 HCAPLUS
CN Silane, [bicyclo[2.2.1]hept-2-ylidene(diethylmethylsilyl)methoxy]diethylme
thyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



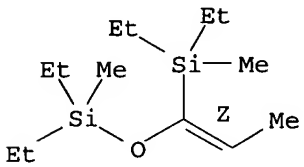
RN 144542-33-6 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-1-propenyl]oxy]diethylmethyl-, (E)- (9CI)
(CA INDEX NAME)

Double bond geometry as shown.

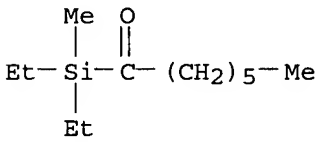


RN 144542-34-7 HCAPLUS
CN Silane, [[1-(diethylmethylsilyl)-1-propenyl]oxy]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

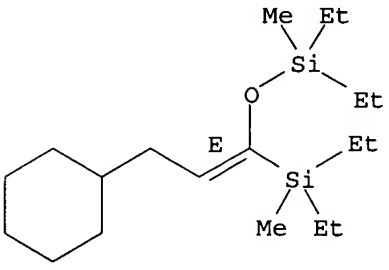


RN 144542-35-8 HCAPLUS
CN Silane, diethylmethyl(1-oxoheptyl)- (9CI) (CA INDEX NAME)



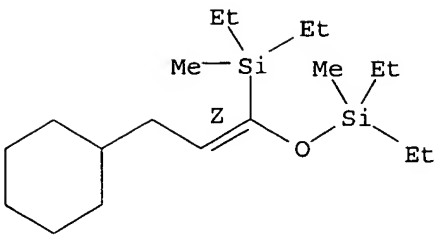
RN 144564-72-7 HCAPLUS
CN Silane, [3-cyclohexyl-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 144564-73-8 HCAPLUS
CN Silane, [3-cyclohexyl-1-[(diethylmethylsilyl)oxy]-1-propenyl]diethylmethyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L64 ANSWER 37 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:496882 HCAPLUS
DOCUMENT NUMBER: 107:96882
TITLE: Novel process for the preparation of halopropyltrialkoxysilanes and halopropylalkylalkoxysilanes
INVENTOR(S): Quirk, Jennifer M.; Kanner, Bernard
PATENT ASSIGNEE(S): Union Carbide Corp., USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4658050	A	19870414	US 1986-846176	19860331
CA 1307287	A1	19920908	CA 1986-524638	19861205
EP 239677	A2	19871007	EP 1986-117784	19861219
EP 239677	A3	19880720		
EP 239677	B1	19900131		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 62230794	A2	19871009	JP 1986-301825	19861219
JP 02057076	B4	19901203		
AT 49974	E	19900215	AT 1986-117784	19861219

PRIORITY APPLN. INFO.: US 1986-846176 A 19860331
EP 1986-117784 A 19861219

AB XCH2CHR2CH2SiRn(OR1)3-n (R,R1 = C1-6 alkyl; R2 = H, C1-6 alkyl; X = Cl, Br, iodide; n = 0-2) are prepared by hydrosilation of allylic halides in the presence of [Ir(L)X]2 catalysts [L = (cyclo)**diene**]. A mixture of HSi(OEt)3 1, allyl chloride 0.5, and xylene 0.5 g was heated at 80° for 4 h in the presence of 0.19 mg [Ir(COD)Cl]2 (COD = 1,5-**cyclooctadiene**) to give 75% ClCH2CH2CH2Si(OEt)3.

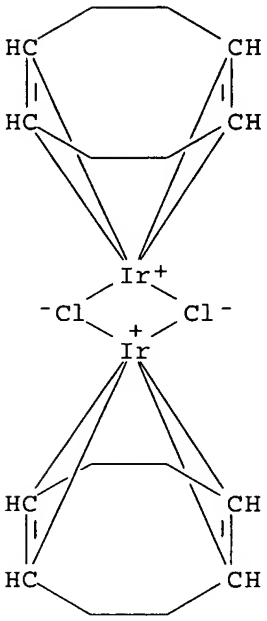
IC ICM C07F007-08
ICS C07F007-18
INCL 556479000
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 67
IT Hydrosilylation catalysts
(iridium **cycloalkadiene** halide dimers, for allylic halides)
IT **12112-67-3**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for hydrosilylation of allyl chloride)
IT **998-30-1**, Triethoxysilane **2031-62-1**, Methyldiethoxysilane **2487-90-3**, Trimethoxysilane **6675-79-2**, Triisopropoxysilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrosilylation by, of allyl chloride)

IT **2530-87-2P**, 3-Chloropropyltrimethoxysilane **5089-70-3P**, 3-Chloropropyltriethoxysilane **13501-76-3P**, 3-Chloropropylmethyldiethoxysilane **61214-14-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by hydrosilylation of allyl chloride)

IT **12112-67-3**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for hydrosilylation of allyl chloride)

RN 12112-67-3 HCAPLUS

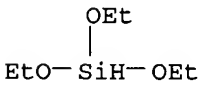
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



IT **998-30-1**, Triethoxysilane **2031-62-1**, Methyldiethoxysilane **2487-90-3**, Trimethoxysilane **6675-79-2**, Triisopropoxysilane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrosilylation by, of allyl chloride)

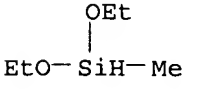
RN 998-30-1 HCAPLUS

CN Silane, triethoxy- (6CI, 8CI, 9CI) (CA INDEX NAME)

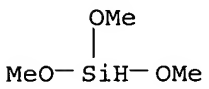


RN 2031-62-1 HCAPLUS

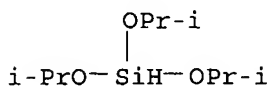
CN Silane, diethoxymethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



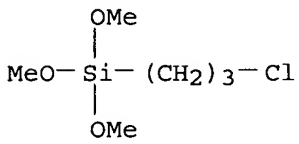
RN 2487-90-3 HCAPLUS
CN Silane, trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



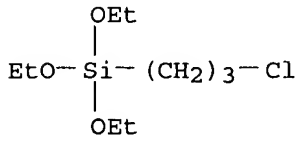
RN 6675-79-2 HCAPLUS
CN Silane, tris(1-methylethoxy)- (9CI) (CA INDEX NAME)



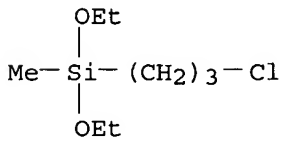
IT **2530-87-2P**, 3-Chloropropyltrimethoxysilane **5089-70-3P**, 3-Chloropropyltriethoxysilane **13501-76-3P**, 3-Chloropropylmethyldiethoxysilane **61214-14-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by hydrosilylation of allyl chloride)
RN 2530-87-2 HCAPLUS
CN Silane, (3-chloropropyl)trimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



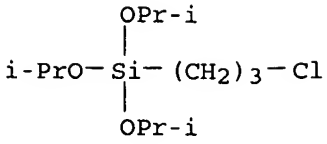
RN 5089-70-3 HCAPLUS
CN Silane, (3-chloropropyl)triethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 13501-76-3 HCAPLUS
CN Silane, (3-chloropropyl)diethoxymethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



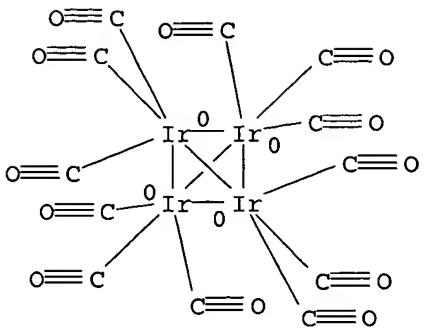
RN 61214-14-0 HCAPLUS
CN Silane, (3-chloropropyl)tris(1-methylethoxy)- (9CI) (CA INDEX NAME)



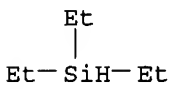
L64 ANSWER 38 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:563243 HCAPLUS
DOCUMENT NUMBER: 97:163243
TITLE: Photoactivated catalytic hydrosilylation of carbonyl compounds
INVENTOR(S): Yates, Ronald L.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4332654	A	19820601	US 1981-284034	19810717
US 4383120	A	19830510	US 1981-320237	19811112

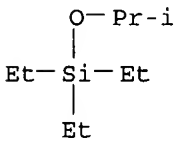
PRIORITY APPLN. INFO.: US 1981-284034 A2 19810717
OTHER SOURCE(S): MARPAT 97:163243
AB Photohydrosilylation of acetone with HSiEt3 gave Me2CHOSiEt3. Transition metal carbonyls, Re2(CO)10, Ir4(CO)12, Os3(CO)12, Ru3(CO)12, LIr(CO)2 (L = acetylacetonate), Fe3(CO)12, Co2(CO)8, Cr(CO)6, Rh6(CO)16, Co2(CO)6(PPh3)2, Co4(CO)12, and Fe2(CO)9, were used as catalysts. Ac(CH2)4Me, cycloheptanone, and PrCHO were also photohydrosilylated with HSiEt3.
IC C07F007-18
INCL 204158000R
CC 29-6 (Organometallic and Organometalloidal Compounds)
IT 10210-68-1 13007-92-6 14023-80-4 14285-68-8 15243-33-1
15321-51-4 15696-40-9 17685-52-8 17786-31-1 **18827-81-1**
24212-54-2 28407-51-4
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for photohydrosilylation of carbonyl compds.)
IT **617-86-7**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(photohydrosilylation of carbonyl compds. with, catalysts for)
IT **1571-45-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT **2751-87-3P 51276-59-6P** 83276-09-9P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
IT **18827-81-1**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalyst, for photohydrosilylation of carbonyl compds.)
RN 18827-81-1 HCAPLUS
CN Iridium, dodecacarbonyltetra-, tetrahedro (9CI) (CA INDEX NAME)



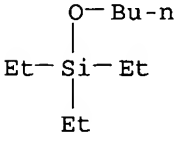
IT **617-86-7**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(photohydrosilylation of carbonyl compds. with, catalysts for)
RN 617-86-7 HCAPLUS
CN Silane, triethyl- (6CI, 8CI, 9CI) (CA INDEX NAME)



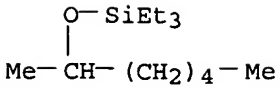
IT **1571-45-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 1571-45-5 HCAPLUS
CN Silane, triethyl(1-methylethoxy)- (9CI) (CA INDEX NAME)



IT **2751-87-3P 51276-59-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 2751-87-3 HCAPLUS
CN Silane, butoxytriethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 51276-59-6 HCAPLUS
CN Silane, triethyl[(1-methylhexyl)oxy]- (9CI) (CA INDEX NAME)



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